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Review of the 1st Watch List under the Water Framework Directive and recommendations for the 2nd Watch List

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Contents

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Executive summary

The surface water Watch List (WL) under the Water Framework Directive (WFD) is a mechanism for obtaining high-quality Union-wide monitoring data on potential water pollutants for the purpose of determining the risk they pose and thus whether Environmental Quality Standards (EQS) should be set for them at EU level. According to the EQS Directive (article 8b)[1], this list should be updated every 2 years.

The main objectives of this report are:

- To present an overview of the data gathered during the 1st year of monitoring of the 1st WL (also called WL dataset in this report),
- To assess whether this WL dataset is sufficient to determine the risk posed by the WL substances, and consequently to determine whether any of these substances can be taken out of the WL,
- To propose new substance(s) to be included in the second WL, using the information and results from the latest review of the list of priority substances, as well as any other relevant information available at the time of this report.

This summary first explains the context for the assessment. Then, mirroring the report itself, it presents an overview of the WL dataset for the different WL substances, it specifies the criteria for taking substances out of the WL and the substances proposed on the basis of these criteria, and finally it presents the criteria for including new substances in the WL and the new proposed WL candidates.

Context of the assessment: Data scenarios, STE score and PNEC (or EQS) used

How to use and interpret non-quantified samples is a challenge when dealing with datasets in which not all limits of quantification (LOQs) are adequate, which is the case in the WL dataset.

To deal with this issue, **3 data scenarios are considered in this report,** as was done during the latest review of the priority substances list (see Carvalho et al, 2016). Scenario 1 (Sc1) includes only quantified samples, thus clearly overestimating the risk. In both Scenario 2 (Sc2) and Scenario 3 (Sc3), non-quantified samples are set to half LOQ[2]. Sc2 comprises all monitoring records, thus leading to non-confirmed exceedances when ½LOQ>PNEC, while Sc3[3] takes into account quantified monitoring samples and non-quantified samples only when ½ LOQ ≤ PNEC (or EQS) (thus avoiding these non-confirmed exceedances)[4]. According to the sub-group on review of the priority substances list (SG-R), Sc3 is the most relevant scenario to assess whether the substance poses a risk at EU-level. In addition, comparing the conclusions made on the basis of Sc2 and Sc3 gives information on the impact of the non-quantified samples on the overall assessment. Therefore these 2 scenarios (Sc2 and Sc3) are used to assess the quality of the WL dataset.

In this report, the preferred indicator for the evaluation of the substances is the STE score, which takes into account the Spatial, Temporal and Extent of exceedances of the

[1] Directive 2008/105/EC, amended by Directive 2013/39/EU.

[2] Under the QA/QC Directive and EQS Directive, MS are required to replace the non-quantified samples by half LOQ to assess compliance with the EQS for individual substances, however the amended EQSD mentions that "when the calculated mean value of a measurement, when carried out using the best available technique not entailing excessive costs, is referred to as "less than limit of quantification", and the limit of quantification of that technique is above the EQS, the result for the substance being measured shall not be considered for the purposes of assessing the overall chemical status of that water body".

[3] Sc3 was called Sc2-PNECQC in the monitoring based prioritisation report (Carvalho et al., 2016).

[4] It should be noted that Sc3 could lead to an underestimation of the risk, if the non-quantified samples with PNEC<LOQ<2PNEC are actually samples where the concentrations exceeds the PNEC.

PNECs. This assessment tool was developed by the JRC for the review of the list of priority substances, with the support of the SG-R.[5]

Two sets of PNECs are considered in the evaluation of WL substances:

- PNECs from the 2015 JRC report entitled "Development of the 1st Watch List under the Environmental Quality Standards Directive" by Raquel N. Carvalho, Lidia Ceriani, Alessio Ippolito and Teresa Lettieri. These will be called the "2015 PNECs".

- updated PNECs, based on the prioritisation exercise and on additional information received from Germany, Switzerland, and Netherlands. These will be called "updated PNECs".

The final assessment, including the recommendation for removal from the watch list, is based on the results obtained with the updated PNECs, whenever available.

WL dataset

The first WL dataset gathers data from 25 EU Member States (MS) with a total number of 35848 surface water samples in Sc2. The vast majority of these records are river water samples (98.3%), with a few measurements for lakes (1.2%) and coastal/transitional waters (0.5%).

For 9 out of 17 substances, the quantification frequency (percentage of quantified samples in Sc2) is below 10%, and for two of them (acetamiprid and methiocarb) below 1%. The quantification frequency for clarithromycin, diclofenac and estrone is above 50%.

Some MS had difficulty in always reaching an analytical LOQ below the 2015 PNECs and/or updated PNECs for 5 (17-alpha-ethinylestradiol, 17-beta-estradiol, azithromycin, imidacloprid, and methiocarb) of the 17 WL substances.

Around half of the MS provided information on the representativity of the monitoring stations and monitoring strategy including the nearby pressures (agricultural, urban, industrial, or recreational / bathing water).

Exceedances of the 2015 PNECs were observed mainly for 17-alpha-ethinylestradiol (EE2), imidacloprid, 17-beta-estradiol (E2), diclofenac, azithromycin, clarithromycin, and estrone (E1). For the other substances there were very few exceedances.

The highest STE scores in Sc3 for WL dataset and PNECs from the WL report 2015 were obtained for: 17-alpha-ethinylestradiol (0.90), imidacloprid (0.69), 17-beta-estradiol (0.65), diclofenac (0.64), estrone (0.54), clarithromycin (0.52), methiocarb (0.45), and azithromycin (0.35).

When using the updated PNEC values with the WL dataset in Sc3, there is on average, a small to medium increase of STE scores for diclofenac, methiocarb, azithromycin and thiacloprid in comparison with the STE scores with PNECs from the WL report 2015.

The analyses of the WL dataset are presented in chapters 2 to 6. In addition the main findings for each substance are shown in a dedicated summary section, after this executive summary.

Review of the 1st WL

As already mentioned above, substances are included in the WL to gather sufficient, high-quality monitoring data to assess the risk they pose at EU level[6]. Consequently, a

[5] For more details about the STE score, please see (Carvalho et al., 2016), available at the following link : https://circabc.europa.eu/sd/a/7fe29322-946a-4ead-b3b9-e3b156d0c318/Monitoring-based%20Exercise%20Report_FINAL%20DRAFT_25nov2016(1).pdf

substance can be taken out of the WL if enough high-quality monitoring data has been collected to allow this risk assessment, otherwise it needs to stay on the list. Whether a substance is shown to pose a significant risk at EU-level or not based on the WL monitoring data is crucial to decide how to deal with the substance once it has been taken off the WL. However, it is not part of the decision to keep or not a substance in the list, on which this report focusses.

The criteria below are intended to identify substances for which there are sufficient, high-quality, EU-wide monitoring data. Please note, however, that this doesn't preclude the possibility of deciding that a substance with monitoring data of a lower quality (not meeting all the criteria below) should be prioritised in a future exercise. Additional evidence (including other monitoring data, information on use, persistence, etc…) could help to provide a sufficient degree of certainty as regards the risk posed by the substance.

In order to judge the collection of high quality monitoring data to assess the EU risk, the JRC proposes the criteria below, assuming a monitoring in appropriate matrix. A substance can be taken out of the WL if it fulfils all criteria simultaneously:

1. The ½ LOQ must be below or equal to the PNEC, for at least 90 % of the non-quantified samples in Sc2 (LOQ-PNEC criterion).
2. Similarity of STE scores for Sc3 and Sc2 (no more than 15% difference in STE scores demonstrating no significant analytical problem with non-quantified samples; the difference of the STE scores is calculated as a percentage by the formula: $|STE_{Sc3} - STE_{Sc2}|/STE_{Sc3} * 100$)

Please note that because of the requirement of the EQSD as regards monitoring for the WL, the data gathered under the WL mechanism is expected to fulfil the minimum requirements in terms of number of MS, sites and samples used during the last prioritisation exercise[7]. This has been checked for each substance, both for scenario 2 and scenario 3.

When considering the WL dataset together with the updated PNECs, the substances fulfilling the 2 above criteria are: diclofenac, clarithromycin, erythromycin, oxadiazon, tri-allate, 2,6-di-tert-butyl-4-methylphenol, acetamiprid, clothianidin, thiacloprid, and 2-ethylhexyl-4-methoxycinnamate.

For information, the same assessment has been carried out on a dataset combining the WL dataset and the dataset used during the review of the priority substances. The conclusions obtained with this combined dataset support the conclusions above (more details are provided in section 7.1 dedicated to removal of substances from the WL).

In addition, it should be noted that:

- Neonicotinoids and macrolide antibiotics were included as groups in the WL, and all substances in each of these groups can be monitored with the same analytical method, so it makes sense to keep them jointly in the WL. In addition, ongoing work at EU-level (see section 7.1 for more details) may lead to a change in the conditions of approval of several of the neonicotinoids, thus possibly leading to substitution effects, and to changes in the risk posed by these substances. Consequently, the data collected so far under the WL may possibly not reflect the risk posed by the substances in the very near future, and it makes sense to keep them in the list to gather sufficient, high quality monitoring data to confirm the risk they pose.

- As regards the sunscreen ingredient 2-ethylhexyl-4-methoxycinnamate, it is unclear how far the monitoring sites selected were representative of the relevant pressure (samples should be taken preferentially in the summer at bathing sites). It is also worth

[6] The EQS Directive also highlights the specific cases of diclofenac and the estrogens, which were put on the WL to "gather monitoring data for the purpose of facilitating the determination of appropriate measures to address the risk posed by those substances."

[7] At least 4 MS, 10 sites and 51 samples.

noting that this substance was initially recommended for monitoring in sediment[8], but that most data received were for water. The few sediment data reported to the JRC were not enough to carry out a conclusive analysis for that matrix. Consideration is being given to including several substances for monitoring in sediment in a WL update in 2019. Therefore we propose to remove the sunscreen ingredient (currently monitored in water) from the current WL in 2018, and to consider its reinclusion in 2019 for sediment monitoring together with the other candidate substances mentioned below. This will ensure the timely and cost-efficient development / validation of analytical methods (in particular by optimising the use of sediment samples) and sediment PNECs.

Overall, based on the above criteria and discussion, the following substances are proposed for removal from the list: diclofenac, oxadiazon, 2,6-di-tert-butyl-4-methylphenol, tri-allate and 2-ethylhexyl-4-methoxycinnamate.

Table 1: Summary information for substances in the 1st WL about PNEC values, fulfilment of removal criteria, and JRC's recommendation on whether to include the substance in the 2nd WL (based on WL dataset and updated PNECs). The fulfilment of the removal criteria of substances and the additional information taken into account for the final decision are described in the chapter 7.1.

Substance	Substance type	PNEC WL 2015 (µg/l)	PNEC update (µg/l)	JRC's Recommendation
17-alpha-Ethinylestradiol (EE2)	Synthetic estradiol hormone	0.000035 (1)		Inclusion in the 2nd WL
17-beta-Estradiol (E2)	Natural female sex hormone	0.0004 (1)		Inclusion in the 2nd WL
Estrone (E1)	Hormone	0.0036 (1)		Inclusion in the 2nd WL
Diclofenac	Non-steroidal anti-inflammatory drug (NSAID)	0.1 (1)	0.05 (4,6)	Removal from the WL
2,6-Di-tert-butyl-4-methylphenol	Antioxidant	3.16 (2)		Removal from the WL
2-Ethylhexyl 4-methoxycinnamate	Sunscreen ingredient / UV filter	6.0 (2) 200 µg/kg (3) (sediment)		Removal from the WL
Erythromycin	Macrolide antibiotic	0.2 (2)		Fulfils both removal criteria but recommended for the 2nd WL
Clarithromycin	Macrolide antibiotic	0.13 (2)	0.12(5)	Fulfils both removal criteria but recommended for the 2nd WL
Azithromycin	Macrolide antibiotic	0.09 (2)	0.019(5)	Inclusion in the 2nd WL
Methiocarb	Carbamate insecticide and herbicide	0.01 (2)	0.002(4,7)	Inclusion in the 2nd WL
Oxadiazon	Herbicide	0.088 (2)		Removal from the WL
Triallate	Herbicide	0.67 (2)	0.41(4)	Removal from the WL
Imidacloprid	Neonicotinoid insecticide	0.009 (2)	0.0083(4)	Inclusion in the 2nd WL
Thiacloprid	Neonicotinoid insecticide	0.05 (2)	0.01(4)	Fulfils both removal criteria but recommended for the 2nd WL
Thiamethoxam	Neonicotinoid insecticide	0.14 (2)	0.042(5)	Inclusion in the 2nd WL
Clothianidin	Neonicotinoid	0.13 (2)		Fulfils both removal criteria but

[8] Recital 9 of Commission Implementing Decision 2015/495: "*For comparability, all substances should be monitored in whole water samples. However, it would be appropriate to monitor 2-ethylhexyl 4-methoxycinnamate also in suspended particulate matter or sediment, because of its tendency to partition into this matrix*."

	insecticide			recommended for the 2nd WL
Acetamiprid	Neonicotinoid insecticide	0.5 (2)		Fulfils both removal criteria but suggested for the 2nd WL

PNECs (or EQS) taken from:

(1) Commission's priority substances proposal from the year 2012 (EU, 2012).

(2) (Carvalho et al. 2015).

(3) Sediment PNEC (Carvalho et al. 2015)

(4) Monitoring-based prioritisation report (Carvalho et al., 2016) https://circabc.europa.eu/w/browse/52c8d8d3-906c-48b5-a75e-53013702b20a)

(5) Oekotoxzentrum Centre Ecotox, 2016

(6) EQS Datasheet, Environmental Quality Standard, Diclofenac, German Environment Agency (UBA), 2017

(7) Ctgb (The Netherlands), 2010. SEC Adviesrapport 12707A01, Methiocarb, Afleiding van het MTR-water. Scheepmaker JWA. 24478-MTR. October 2010.

Selection of new substances for the 2nd WL

According to the EQS Directive, the total number of substances/groups of substances in the WL can increase by one at each update of the list, up to 14 substances, meaning that the 2nd WL can include up to 11 (groups of) substances. Candidate WL substances should be selected among substances posing a potential risk for the environment, but for which there is not enough good quality monitoring data to confirm this risk. A reliable PNEC and an appropriate analytical method (LOQ at least as low as the PNEC) should be available for new substances included in the WL.

The criteria proposed here for identifying new WL substances generally follow the approach adopted in the 1st WL report (Carvalho et al., 2015) and build on the technical work carried out for the review of the priority substances list led by the JRC with the support of the SG-R. During the review, substances with enough monitoring data to assess the risk they posed went through the so-called "monitoring-based approach", while others went through the modelling-based approach. Factsheets were drafted for substances ranking high through either of these approaches. On the basis of these factsheets, 10 substances were short-listed for further consideration.

For more details on the methodologies, please see the summary available at the following link: https://circabc.europa.eu/w/browse/0f6b893e-b0ab-46cb-a631-c3e1e55c7514

Consequently, the JRC suggests the following criteria for the selection of new substances as potential candidates for the WL:

Criteria based on the 2014 prioritisation:

1. Substances for which factsheets were prepared during the prioritisation process but not taken forward because there were few or low-quality monitoring data.
2. Substances short-listed but with uncertainties in the monitoring data,
3. Substances considered in the modelling based exercise for which:
    a. The monitoring data met the representativity criteria (number of MS, sites and samples) in Sc2 but not in Sc3, AND
    b. In Sc2 the STE score was high and the modelled RQ was high.
4. Substances considered in the prioritisation exercise which went directly to the modelling exercise (measured in less than 4 MS in Sc2) with a modelled RQ above 5, but not further selected because of lack of monitoring data.

Additional criteria:

5. Substances identified as potentially relevant in the report "Development of the first Watch List" (Carvalho, et al., 2015), but not included in the 1st WL because of limitations in the information available at the time (e.g. on analytical methods).

6. Substances of emerging concern identified based on research projects and scientific articles, in line with the requirement of EQSD article 8b.

Substances fulfilling these criteria that could be considered for inclusion in the WL depending on the availability of a reliable PNEC and appropriate analytical methods, are (see section 7.2 for more details):

- Criterion 1: chromium (VI) (dissolved)

- Criterion 2: permethrin, esfenvalerate, deltamethrin and bifenthrin,

- Criterion 3 and 4: diflubenzuron, pyridaben, dimoxystrobin, etofenprox, fenpyroximate, metaflumizone, proquinazide, and venlafaxine,

- Criterion 5: free cyanide (CN^-)

- Criterion 6: the antibiotics amoxicillin and ciprofloxacin. The selection of these antibiotics is also in line with the European One Health Action Plan against antimicrobial resistance[9].

Taking into account the availability of an appropriate analytical method (LOQ at least as low as the PNEC) and of a reliable PNEC, the JRC recommends the inclusion of metaflumizone, amoxicillin and cyprofloxacin in the 2nd WL.

High modelled RQ substances such as the pyrethroids (etofenprox, permethrin, esfenvalerate, deltamethrin and bifenthrin) and pyridaben should be considered in the 3rd WL, however, based on their physical chemical properties, they should be measured in the most relevant matrix, i.e. sediment or biota (the PNEC and analytical methods would still need to be investigated). Furthermore venlafaxine and proquinazid should be also considered for the 3rd WL if reliable information for the PNEC is found. Free cyanide should also be considered when the analytical method recently developed is made available. The review of approval of dimoxystrobin is due by January 2019. If the approval for this substance is renewed, then it can be considered for inclusion in the 3rd WL. No appropriate analytical method has been found for diflubenzuron and fenpyroximate.

Chromium (VI) is not proposed for inclusion in the 2nd WL. The JRC's assessment of the new monitoring data received in January 2018 together with the data from the 2014 prioritisation doesn't support the idea that chromium (VI) would be posing a risk in freshwaters. However, chromium (VI) could be considered for inclusion in the 3rd watch list in transitional and coastal waters, after confirmation of the PNEC via consultation with the WG Chemicals and after collection and analysis of any additional existing monitoring data for these categories of water.

Finally, thiram, metconazole and famoxadone could be considered for inclusion in the 3rd WL if their approval is renewed and if a reliable PNEC and an appropriate analytical method are found.

Table 11 summarizes the availability of reliable PNECs and appropriate analytical methods for the above-mentioned substances.

[9] https://ec.europa.eu/health/amr/sites/amr/files/amr_action_plan_2017_en.pdf
The Action Plan states: "maximise the use of data from existing monitoring, e.g. Watch List monitoring under the Water Framework Directive, to improve knowledge of the occurrence and spread of antimicrobials in the environment"

Summary of most important findings for the WL substances

The findings and conclusions on the removal from the WL (or inclusion in the 2nd WL) are based on the WL dataset and both sets of PNEC values (from 2015 and updated). In the following tables all concentrations are given in µg/l.

17-alpha-Ethinylestradiol (EE2)

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	EQS	Median	Mean	P95	Max
Sc1	10	54	82	100	0.000035	**0.00010**	0.00023	0.00078	0.0030
Sc2	25	224	558	14.7		**0.00005**	0.00055	0.0010	0.0125
Sc3	14	123	323	25.4		0.000015	0.00007	0.00026	0.0030

The European median surface water concentration of EE2 is higher than the EQS (0.035 ng/l) in the data scenarios Sc1 (0.1 ng/l) and Sc2 (0.05 ng/l), but lower in Sc3 (0.015 ng/l).

Note that from the 82 quantified samples 75 exceed the EQS of 0.000035 µg/l, and 7 samples were given as 0.00003 µg/l.

241 of the 476 non-quantified samples are below the EQS but still very close because the lowest reported LOQ was 0.00003 µg/l. 235 of the non-quantified samples are above the EQS but are removed in Sc3 because the LOQ is not sufficient.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.899	1.910	2.191	7.4	28.6	22.3

General information on data quality

In Sc2 558 samples from 25 countries are available (quantification frequency 14.7 %), and in Sc3 323 samples from 14 countries.

A detailed analysis of the LOQs for the non-quantified samples showed that 4 MS achieved an LOQ of 0.03 ng/l (for 172 samples) which is below the EQS (0.035 ng/l). Other 4 countries reached an LOQ of 0.035 ng/l (for 57 samples), equal to the EQS; 4 other countries have an LOQ of 0.1 ng/l (for 70 samples). There are however 12 countries with an LOQ clearly not sufficient for the low EQS of 0.035 ng/l (for 247 samples).

Assessment of removal criteria and conclusion as regards removal

Data quality for EE2 is not satisfactory because 12 MS don't achieve the low EQS of EE2. The ½ LOQ is ≤ EQS for only 50.6 % of the non-quantified samples in Sc2 (threshold=90%).

The STE score of Sc2 is much higher than for Sc3 (the difference is above the limit of 15 %).

EE2 should remain on the WL.

17-beta-Estradiol (E2)

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	EQS	Median	Mean	P95	Max
Sc1	11	60	101	100	0.0004	0.00021	0.00041	0.00130	0.0030
Sc2	25	229	597	16.9		0.00017	0.00059	0.00150	0.0125

Sc3	18	181	461	21.9		0.00015	0.00020	0.00051	0.0030

The European median surface water concentration of E2 is in all data scenarios below the EQS (0.4 ng/l).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.646	1.165	1.090	1.3	3.8	3.3

General information on data quality

In Sc2 597 samples from 25 countries are available (quantification frequency 16.9 %), and in Sc3 461 samples from 18 countries. For E2 most non-quantified samples have an LOQ ≤ the EQS of 0.4 ng/l (360 out of 497 samples). The LOQs range from 0.03 – 25 ng/l. There are 16 countries which achieve with their analytical method the EQS of E2, and 8 countries with higher LOQs.

Assessment of removal criteria and conclusion as regards removal

Data quality for E2 is not satisfactory because several MS don't achieve the EQS. However, the ½ LOQ is ≤ EQS for 72.8 % of the non-quantified samples in Sc2, which is below the threshold of 90 %.

The STE scores of Sc2 and Sc3 are different (the difference is > 15 %).

E2 should remain on the WL.

Estrone (E1)

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	13	141	313	100	0.0036	0.00064	0.0015	0.0050	0.031
Sc2	23	213	574	54.5		0.00050	0.0013	0.0050	0.031
Sc3	20	198	552	56.7		0.00050	0.0010	0.0035	0.031

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.542	0.796	0.672	0.97	1.39	1.39

General information on data quality

In Sc2 574 samples from 23 countries are available (quantification frequency 54.5 %), and in Sc3 552 samples from 20 countries. Most of the countries achieve the PNEC of E1; there are only 22 samples from 4 countries with an LOQ > PNEC.

Assessment of removal criteria and conclusion as regards removal

Data quality for E1 is relatively good; however only one of the two removal criteria is fulfilled.

Most of the countries achieve the PNEC. The ½ LOQ is ≤ PNEC for 91.6 % of the non-quantified samples in Sc2.

The STE scores are similar but not identical; the difference is > 15 % (47 %).

E1 should remain on the WL.

Diclofenac

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	21	529	4602	100	0.1	0.047	0.093	0.34	2.6
Sc2	25	608	6698	68.7		0.027	0.067	0.26	2.6
Sc3	25	608	6697	68.7		0.027	0.067	0.26	2.6

The median concentration of diclofenac is between 0.027 µg/l (Sc3 and Sc2) and 0.047 µg/l (Sc1).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.645	0.645	0.864	2.6	2.6	3.4

For diclofenac a lower PNEC of 0.05 µg/l has been derived in the finalised dossier from Germany, which results in increased STE scores and RQs.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.990	0.990	1.335	5.3	5.3	6.8

General information on data quality

In Sc2 6698 samples from 25 countries are available (quantification frequency 68.7 %), and in Sc3 6697 samples from 25 countries, so that the data quality is very good. All laboratories achieve the PNEC (the ½ LOQ is ≤ PNEC for all but one of the non-quantified samples in Sc2). The STE scores of Sc2 and Sc3 are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for diclofenac is good; both removal criteria are fulfilled.

There is no need to collect additional monitoring data for this substance in the WL.

Diclofenac can be removed from the WL.

2,6-Di-tert-butyl-4-methylphenol

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	6	22	57	100	3.16	0.018	0.512	0.26	14.0
Sc2	24	245	1035	5.5		0.0050	0.10	0.25	14.0
Sc3	23	242	1032	5.5		0.0050	0.088	0.25	14.0

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.167	0.000	0.08	0.08	0.08

General information on data quality

In Sc2 1035 samples from 24 countries are available (quantification frequency 5.5 %), and in Sc3 1032 samples from 23 countries. Nearly all LOQs are below the PNEC; there are 3 samples with an LOQ of 9 µg/l, and 10 samples with an LOQ equal to the PNEC (3.16 µg/l). The ½ LOQ is ≤ PNEC for 99.7 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are not identical, but the datasets of Sc2 and Sc3 are nearly identical. [10]

Assessment of removal criteria and conclusion as regards removal

Data quality for 2,6-di-tert-butyl-4-methylphenol is good; both removal criteria are fulfilled.

2,6-Di-tert-butyl-4-methylphenol can be removed from the WL.

2-Ethylhexyl 4-methoxycinnamate

Statistics on samples, concentrations, STE scores and RQs

2-Ethylhexyl 4-methoxycinnamate is a sunscreen ingredient / UV filter with a water PNEC of 6.0 µg/l and a sediment PNEC of 200 µg/kg.

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	6	19	116	100	6.0	0.305	0.420	1.4	1.8
Sc2	24	201	546	21.2		0.050	0.367	3.0	9.0
Sc3	23	198	543	21.4		0.050	0.319	3.0	3.0

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	0.000	0.50	0.50	0.23

General information on data quality

In Sc2 546 samples from 24 countries are available (quantification frequency 21.2 %), and in Sc3 543 samples from 23 countries. Nearly all LOQs are below the PNEC; there are 3 samples with an LOQ of 18 µg/l, and 33 samples with an LOQ equal to the PNEC (6 µg/l). The ½ LOQ is ≤ PNEC for 99.3 % of the non-quantified samples in Sc2.

The STE scores are identical.

Sediment analysis

In sediment 2-ethylhexyl-4-methoxycinnamate was analysed in 4 countries with a total number of samples of 37. No nearby pressure information (bathing site) was given. The maximum concentration detected for 2-ethylhexyl-4-methoxycinnamate in sediment was 35 µg/kg, and therefore did not exceed the PNEC of 200 µg/kg.

Assessment of removal criteria and conclusion as regards removal

Data quality for 2-ethylhexyl 4-methoxycinnamate in water is good; both removal criteria are fulfilled.

However, the number of samples in sediment is very low, and better nearby pressure information (bathing water) would be needed; 2-ethylhexyl 4-methoxycinnamate should be monitored in sediment during the summer at bathing sites; therefore, it is proposed to remove 2-ethylhexyl 4-methoxycinnamate from the current WL and to consider its reinclusion in 2019 for sediment monitoring.

[10] When STE_{Sc3}=0 and STE_{Sc2} is very low (<0.2 or =0) the difference of these scores is assumed to be zero (see section 7.1).

Erythromycin

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	12	89	211	100	0.2	0.026	0.060	0.20	1.1
Sc2	24	300	2520	8.4		0.0050	0.012	0.028	1.1
Sc3	19	277	2491	8.5		0.0050	0.012	0.028	1.1

The median concentration of erythromycin is between 0.005 (Sc3 and Sc2) and 0.026 µg/l (Sc1).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	0.480	0.14	0.14	1.00

General information on data quality

In Sc2 2520 samples from 24 countries are available (quantification frequency 8.4 %), and in Sc3 2491 samples from 19 countries. Nearly all LOQs are below the PNEC; there are only 2 samples with an LOQ equal to the PNEC (0.2 µg/l). The ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2.

The STE scores are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for erythromycin is good; both removal criteria are fulfilled.

However the JRC proposes to continue monitoring it together with the other macrolide antibiotics.

Clarithromycin

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	17	201	1642	100	0.13	0.034	0.073	0.28	1.6
Sc2	24	324	2792	58.8		0.016	0.047	0.17	1.6
Sc3	24	324	2792	58.8		0.016	0.047	0.17	1.6

The median concentration of clarithromycin is between 0.016 (Sc3 and Sc2) and 0.034 µg/l (Sc1).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.515	0.515	0.593	1.34	1.34	2.15

For clarithromycin a slightly lower PNEC of 0.12 µg/l has been proposed by Oekotoxzentrum (CH).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.525	0.525	0.593	1.45	1.45	2.33

General information on data quality

In Sc2 and Sc3 2792 samples from 24 countries are available (quantification frequency 58.8 %). The LOQs of all samples are < PNEC; the ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2.

The STE scores are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for clarithromycin is good; both removal criteria are fulfilled.

However the JRC proposes to continue monitoring it together with the other macrolide antibiotics.

Azithromycin

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	14	75	265	100	0.09	0.023	0.062	0.25	1.0
Sc2	24	288	1553	17.1		0.022	0.030	0.055	5.0
Sc3	19	192	915	29.0		0.022	0.023	0.053	1.0

The median concentration of azithromycin is between 0.022 (Sc3 and Sc2) and 0.023 µg/l (Sc1).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.348	0.351	0.720	0.59	0.61	2.8

For azithromycin a lower PNEC of 0.019 µg/l has been proposed by Oekotoxzentrum (CH), which changes the STE scores strongly.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.879	1.403	1.569	4.5	2.9	13.1

General information on data quality

In Sc2 1553 samples from 24 countries are available (quantification frequency 17.1 %), and in Sc3 915 samples from 19 countries. The LOQ is for most of the samples below the PNEC (0.09 µg/l); only 2 samples have an LOQ of 10 µg/l, and 9 samples and LOQ of 0.1 µg/l (close to the PNEC). The ½ LOQ is ≤ PNEC for 99.8 % of the non-quantified samples in Sc2.

The STE scores are similar in Sc2 and Sc3 (the difference is < 15 %).

Assessment of removal criteria and conclusion as regards removal

Data quality for azithromycin is good; both removal criteria are fulfilled.

However, a lower PNEC of 0.019 µg/l has been proposed for azithromycin which requires lower LOQs in around half of the laboratories. The STE scores for this lower PNEC of 0.019 µg/l are different (the difference is > 15 %).

Therefore azithromycin should remain on the WL.

Methiocarb

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	2	4	6	100	0.01	0.028	0.040	0.090	0.109
Sc2	24	369	1834	0.3		0.0050	0.0061	0.010	0.109
Sc3	7	56	1798	4.7		0.0050	0.0059	0.010	0.109

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.445	0.908	n.a.	1.0	1.0	n.a.

General information on data quality

In Sc2 1834 samples from 24 countries are available (quantification frequency 0.3 %), and in Sc3 1798 samples from 7 countries. In most countries and samples the LOQ is equal to the PNEC (0.01 µg/l). The ½ LOQ is ≤ PNEC for 98 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are different (the difference is > 15 % (104 %)).

Assessment of removal criteria and conclusion as regards removal

Data quality for methiocarb is not satisfactory because the STE scores are different.

Methiocarb should remain on the WL to improve the data quality including better information on nearby pressure (pesticide use information).

In addition, a considerably lower PNEC of 0.002 µg/l was proposed by the Netherlands, which changes the STE scores substantially.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
1.200	1.786	n.a.	0.83	5.0	45.0

Note that nearly all LOQs are above this PNEC.

Imidacloprid

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	15	123	421	100	0.009	**0.018**	0.031	0.082	1.05
Sc2	24	376	2385	17.7		0.0050	0.011	0.027	1.05
Sc3	22	326	1845	22.8		0.0050	0.011	0.033	1.05

The median concentration of imidacloprid exceeds its PNEC (0.009 µg/l) only in Sc1 (0.018 µg/l), but not in Sc2 (0.005 µg/l), or Sc3 (0.005 µg/l).

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.690	1.007	2.005	3.7	3.0	9.1

A slightly lower PNEC of 0.0083 µg/l was available from the prioritisation exercise, which changes the STE scores and RQs only very little.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.753	1.033	2.021	4.1	3.2	9.9

General information on data quality

In Sc2 2385 samples from 24 countries are available (quantification frequency 17.7 %), and in Sc3 1845 samples from 22 countries. The LOQs for imidacloprid range between

0.0006 - 0.05 µg/l. Most of the countries have reported for most of their samples an LOQ of 0.009 µg/l (123 samples in 8 countries) or 0.01 µg/l (1070 samples in 8 countries) which is equal (or nearly equal) to the proposed PNEC of 0.009 µg/l. There are however 11 laboratories (note that some MS report different LOQs from different laboratories) with 687 samples which do not achieve the PNEC. The ½ LOQ is ≤ PNEC for 72.5 % of the non-quantified samples in Sc2, which is below the threshold of 90 %.

The STE scores of Sc2 and Sc3 are different (the difference is > 15 % (37.8 %)).

Assessment of removal criteria and conclusion as regards removal

Data quality for imidacloprid is not satisfactory because the STE scores of Sc2 and Sc3 are different (the difference is > 15 %).

Imidacloprid should remain on the WL.

Thiacloprid

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	12	50	97	100	0.05	0.015	0.026	0.079	0.57
Sc2	24	374	2243	4.3		0.0050	0.0068	0.010	0.57
Sc3	23	366	2235	4.3		0.0050	0.0068	0.010	0.57

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	0.469	0.20	0.20	1.58

General information on data quality

In Sc2 2243 samples from 24 countries are available (quantification frequency 4.3 %), and in Sc3 2235 samples from 23 countries. Nearly all LOQs are below the PNEC; there are only 2 samples with an LOQ equal to the PNEC (0.05 µg/l). The ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are identical.

For thiacloprid a much lower PNEC of 0.01 µg/l has been proposed by Oekotoxzentrum (CH), which would increase the STE scores.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.240	0.251	1.666	1.0	1.0	7.9

Assessment of removal criteria and conclusion as regards removal

Data quality for thiacloprid is good; both removal criteria are fulfilled.

However the JRC proposes to continue its monitoring as explained in section 7.1.

The proposed lower PNEC of 0.01 µg/l would require lower LOQs in several MS laboratories (559 samples).

Thiamethoxam

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	10	67	256	100	0.14	0.015	0.032	0.123	0.77
Sc2	24	418	4020	6.4		0.0050	0.0076	0.013	0.77
Sc3	23	412	3979	6.4		0.0050	0.0076	0.013	0.77

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.062	0.062	0.227	0.09	0.09	0.88

General information on data quality

In Sc2 4020 samples from 24 countries are available (quantification frequency 6.4 %), and in Sc3 3979 samples from 23 countries. The LOQs of all samples are < PNEC; the ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are identical.

For thiamethoxam a lower PNEC of 0.042 µg/l has been proposed by Oekotoxzentrum (CH), which changes the STE scores slightly.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.076	0.300	0.391	0.24	0.30	2.9

Assessment of removal criteria and conclusion as regards removal

Data quality for thiamethoxam with the higher PNEC of 0.14 µg/l is good; both removal criteria are fulfilled. However, the STE scores are not identical with the lower PNEC of 0.042 µg/l (the difference is > 15 %).

Thiamethoxam should remain on the WL.

Clothianidin

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	6	47	217	100	0.13	0.016	0.044	0.173	0.78
Sc2	24	343	2254	9.6		0.0050	0.011	0.033	0.78
Sc3	24	343	2254	9.6		0.0050	0.011	0.033	0.78

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.286	0.286	0.309	0.25	0.25	1.33

General information on data quality

In Sc2 and Sc3 2254 samples from 24 countries are available (quantification frequency 9.6 %). All LOQs are below the PNEC (the ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2), and the STE scores of Sc2 and Sc3 are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for clothianidin is good; both removal criteria are fulfilled.

However the JRC proposes to continue its monitoring as explained in section 7.1.

Acetamiprid

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	7	10	15	100	0.5	0.0090	0.014	0.045	0.074
Sc2	24	372	2221	0.7		0.0050	0.0067	0.010	0.074
Sc3	24	372	2221	0.7		0.0050	0.0067	0.010	0.074

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	n.a.	0.02	0.02	n.a.

General information on data quality

In Sc2 and Sc3 2221 samples from 24 countries are available (quantification frequency 0.7 %). The LOQs of all samples are < PNEC. The ½ LOQ is ≤ PNEC for 100 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for acetamiprid is good; both removal criteria are fulfilled.

However the JRC proposes to continue its monitoring as explained in section 7.1.

Oxadiazon

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	5	17	77	100	0.088	0.010	0.023	0.071	0.31
Sc2	24	339	1849	4.2		0.0050	0.011	0.040	0.31
Sc3	23	337	1847	4.2		0.0050	0.011	0.040	0.31

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.100	0.101	0.450	0.45	0.45	0.80

General information on data quality

In Sc2 1849 samples from 24 countries are available (quantification frequency 4.2 %), and in Sc3 1847 samples from 23 countries. Nearly all LOQs are below the PNEC; there are 2 samples with an LOQ of 0.2 µg/l, and 41 samples with an LOQ of 0.09 µg/l. The ½ LOQ is ≤ PNEC for 99.9 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for oxadiazon is good; both removal criteria are fulfilled.

Oxadiazon can be removed from the WL.

Tri-allate

Statistics on samples, concentrations, STE scores and RQs

Scenario	Countries	Sites	Samples	Quant. Samples (%)	PNEC	Median	Mean	P95	Max
Sc1	4	23	138	100	0.67	0.022	0.037	0.113	0.270
Sc2	24	338	2169	6.4		0.0050	0.015	0.035	0.945
Sc3	23	335	2166	6.4		0.0050	0.014	0.033	0.335

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	0.000	0.05	0.05	0.17

For tri-allate a lower PNEC of 0.41 µg/l was available from the prioritisation exercise, which does not change the STE scores.

STE score			RQ (P95)		
Sc3	Sc2	Sc1	Sc3	Sc2	Sc1
0.000	0.000	0.000	0.08	0.09	0.28

General information on data quality

In Sc2 2169 samples from 24 countries are available (quantification frequency 6.4 %), and in Sc3 2166 samples from 23 countries. Nearly all LOQs are below the PNEC; there are 3 samples with an LOQ of 1.89 µg/l, and 9 samples with an LOQ equal to the PNEC (0.67 µg/l). The ½ LOQ is ≤ PNEC for 99.9 % of the non-quantified samples in Sc2.

The STE scores of Sc2 and Sc3 are identical.

Assessment of removal criteria and conclusion as regards removal

Data quality for tri-allate is good; both removal criteria are fulfilled.

Tri-allate can be removed from the WL.

1. Introduction

The Water Framework Directive's (WFD) surface water Watch List (WL) mechanism was established in 2013 under the Priority Substances Directive 2008/105/EC (as amended by Directive 2013/39/EU). The WL is a mechanism to gather high-quality Union-wide monitoring data for the purpose of supporting future prioritisation exercises by investigating whether the selected chemicals pose a significant risk across the European Union's river basins.

The first WL was established by Commission Implementing Decision (EU) 2015/495 in March 2015. It includes 10 substances or groups of substances (amounting to 17 individual substances) which must be monitored by the EU Member States (MS) at least once annually at a minimum number of monitoring sites in each country. Substances may remain on the WL for up to four years at a stretch, but may be removed sooner, even after only one year, if a decision can already be made on the level of risk they pose. At that point, they could be identified as not posing a significant risk at EU-level (although they could still be relevant at national or river-basin level) or be prioritised for inclusion under WFD as priority substances (EU, 2015).

The first year of WL monitoring began six months after the list was established (therefore on 20th September 2015), and MS had to report the results to the European Commission (EC) by December 2016.

The 10 substances/groups of substances included in the first WL are shown in Table 2, together with their CAS numbers, substance type, and corresponding Predicted No Effect Concentration (PNEC) or Environmental Quality Standard (EQS). The table also presents the recent update of PNEC (or EQS) values, including the source of these proposals, for 9 WL substances.

The first WL includes 3 groups of substances: a group of two natural hormones, five neonicotinoid insecticides, and three macrolide antibiotics. For the group of neonicotinoid insecticides (code EEA_33-52-3) and macrolide antibiotics (code EEA_33-51-2) all MS provided the analytical results for the individual substances and not for the sum of group of substances.

In this report WL substances are evaluated using STE (Spatial, Temporal and Extent of PNEC exceedance) assessment tool (STE is shortly explained in Annex 1) considering two sets of PNEC values:

- PNECs from the 2015 JRC report entitled "Development of the 1st Watch List under the Environmental Quality Standards Directive" by Raquel N. Carvalho, Lidia Ceriani, Alessio Ippolito and Teresa Lettieri. These will be called the "2015 PNECs"

- updated/revised PNECs, coming from the last prioritisation exercise and/or the additional information received from Switzerland, Germany, and the Netherlands. These will be called "updated PNECs".

Thereafter, following the established practice in chemical risk assessment (Carvalho et al., 2016), three data scenarios were considered when the STE model was run (see details in Table 3). Scenario 1 (Sc1) includes only quantified samples while Scenario 2 (Sc2) comprises all monitoring records. In Sc2 the non-quantified samples were set equal to half of LOQ as stipulated in Directive 2009/90/EC. The scenario indicated as Sc3 (quantified monitoring samples plus non-quantified when ½ LOQ ≤ PNEC) actually was called Sc2-PNEC-QC in the monitoring based prioritisation report (Carvalho et al., 2016). The so-called "PNEC quality criteria" reduces the Sc2 data set to the Sc3 subset by removing the non-quantified records which are above the limit of 2*PNEC. However, according to the decisions of the SG-R (sub-group on revision of the priority substances list), Sc3 was deemed to be the most relevant scenario to consider during the prioritisation and the one being the basis for the decisions taken. Following this concept the WL substances were also evaluated using Sc3 data subset.

Table 2: Watch list substances with CAS and PNEC values.

Substance	Substance type	CAS	PNEC WL 2015 (µg/L)	PNEC update (µg/L)
17-alpha-Ethinylestradiol (EE2)	Synthetic estradiol hormone	57-63-6	0.000035 [1]	
17-beta-Estradiol (E2)	Natural female sex hormone	50-28-2	0.0004 [1]	
Estrone (E1)	Hormone	53-16-7	0.0036 [1]	
Diclofenac	Non-steroidal anti-inflammatory drug (NSAID)	15307-86-5	0.1 [1]	0.05 [4,6]
2,6-Di-tert-butyl-4-methylphenol	Antioxidant	128-37-0	3.16 [2]	
2-Ethylhexyl 4-methoxycinnamate	Sunscreen ingredient / UV filter	5466-77-3	6.0 [2] 200 µg/kg [3] (sediment)	
Erythromycin	Macrolide antibiotic	114-07-8	0.2 [2]	
Clarithromycin	Macrolide antibiotic	81103-11-9	0.13 [2]	0.12 [5]
Azithromycin	Macrolide antibiotic	83905-01-5	0.09 [2]	0.019 [5]
Methiocarb	Carbamate insecticide and herbicide	2032-65-7	0.01 [2]	0.002 [4,7]
Oxadiazon	Herbicide	19666-30-9	0.088 [2]	
Triallate	Herbicide	2303-17-5	0.67 [2]	0.41 [4]
Imidacloprid	Neonicotinoid insecticide	105827-78-9 /138261-41-3	0.009 [2]	0.0083 [4]
Thiacloprid	Neonicotinoid insecticide	111988-49-9	0.05 [2]	0.01 [4]
Thiamethoxam	Neonicotinoid insecticide	153719-23-4	0.14 [2]	0.042 [5]
Clothianidin	Neonicotinoid insecticide	210880-92-5	0.13 [2]	
Acetamiprid	Neonicotinoid insecticide	135410-20-7 /160430-64-8	0.5 [2]	

PNECs taken from:

[1] Commission's priority substances proposal from the year 2012 (EU, 2012).

[2] (Carvalho et al. 2015).

[3] Sediment PNEC (Carvalho et al. 2015)

[4] Monitoring-based prioritisation report (Carvalho et al., 2016) https://circabc.europa.eu/w/browse/52c8d8d3-906c-48b5-a75e-53013702b20a)

[5] Oekotoxzentrum Centre Ecotox, 2016

[6] EQS Datasheet, Environmental Quality Standard, Diclofenac, German Environment Agency (UBA), 2017

[7] Ctgb (The Netherlands), 2010. SEC Adviesrapport 12707A01, Methiocarb, Afleiding van het MTR-water. Scheepmaker JWA. 24478-MTR. October 2010.

Table 3: Data scenarios used to score substances with the STE method. The scenario indicated as Sc3, actually was called Sc2-PNEC-QC in the monitoring based prioritisation exercise (Carvalho et al., 2016).

Data scenario	**Description**
Scenario 1 (Sc1)	Only quantified monitoring samples
Scenario 2 (Sc2)	All monitoring samples (quantified and non-quantified). In Sc2 the non-quantified samples were set equal to half of LOQ as stipulated in Directive 2009/90/EC
Scenario 3 (Sc3)	Quantified monitoring samples plus non-quantified when ½ LOQ ≤ PNEC (or EQS) (worked out from Sc2 by applying PNEC quality criterion to the non-quantified samples)

In the last prioritisation exercise a set of minimum representativity criteria were used to determine whether sufficient monitoring data were available to carry out an STE analysis: at least 51 samples should be available from minimum 10 sites and at least 4 MS. Since the WL dataset comprises a considerable amount of measurements from almost all MS, expectedly the aforementioned criteria were always fulfilled in Sc2 and Sc3 (for details see Annex 3).

The purpose of this report is to:

- present an overview of the data gathered during the 1st year of monitoring of the 1st WL (also called WL dataset in this report),
- assess whether this WL dataset is sufficient to determine the risk posed by the WL substances, and consequently to determine whether any of these substances can be taken out of the WL,
- **propose new substance(s) to be included in the second WL**, using the information and results from the latest review of the list of priority substances, as well as any other relevant information available at the time of this report.

Chapters 2 to 6 present the analysis of the 1st year of monitoring data for the first WL. More precisely chapter 2 starts with a presentation of the WL dataset including general information and basic statistical analyses for the number of sites and samples. Chapter 3 continues with the additional analyses for WL dataset on the number of WL substances measured per country, months with measurements in each MS, the frequency of sampling and the nearby pressure information. Chapter 4 shows findings on the data quality. Chapter 5 presents the measured concentrations of WL substances comparing to both sets of PNEC values (from 2015 and updated ones). Then, the STE scores of WL substances are shown in chapter 6 calculated using the WL dataset.

Chapter 7 (discussion) shows the review of the 1st WL and proposals for the second WL. Section 7.1 presents the criteria for the removal of a substance from the WL, and their implementation, leading to the proposed delisting of several of the substances currently in the 1st WL. Section 7.2 presents the criteria for adding new substances in the second WL, and the substances proposed on the basis of these criteria.

The report includes also 9 annexes that show all supportive information in graphical or tabular form.

2. General analysis of WL dataset

The EU Member States (MS) provided the WL monitoring data (mainly for surface water, to a limited extent for sediment) to the Commission by uploading them to the EEA WISE system using the new SoE (State of Environment) reporting template. All countries used the SoE data template for data submission.

Most MS submitted data by the December 2016 deadline, but 3 MS - Spain (ES), Greece (EL), and Malta (MT) did not submit any monitoring records even by a later cut-off date (18 April 2017), put in place to allow timely analysis of the results and timely production of this report. However, if these countries report their disaggregated data for the 1st year of monitoring together with their data for the 2nd year of monitoring, ie by December 2018, they will be used in the production of the next WL report. One EFTA country also proposed data, but only from one monitoring station and for 9 of WL substances (in total 4717 samples). These data were excluded from the statistics for first WL in order to avoid "skewing" the results.

In the individual country's data sets submitted via the SoE data template, all non-quantified samples (< LOQ) were reported as equal to LOQ, in line with the requirements of the data dictionary http://dd.eionet.europa.eu/datasets/latest/WISE-SoE_WaterQuality. These non-quantified samples are set for the statistics and STE runs as half of their LOQ (LOQ/2) according to Directive 2009/90/EC (EU, 2009).

Five MS submitted monitoring data for sediment and one for suspended particulate matter (SPM). A summary of these data is presented in Annex 2. Substances detected in sediment were 2-ethylhexyl-4-methoxycinnamate (countries #07, #09 and #29), clarithromycin (detected only in the country #06; it was analysed in 2 MS), and diclofenac (only once detected in the country #06; analysed in 2 MS). Country #6 analysed clarithromycin, diclofenac, erythromycin, and triallate in SPM, but only clarithromycin was detected. Thus, the sediment and SPM data were not considered in the STE (Spatial, Temporal and Extent of PNEC exceedance) assessment since they do not fulfil the minimum representativity criteria (sufficient number of countries, sites and samples). The maximum concentration detected for 2-ethylhexyl-4-methoxycinnamate in sediment was 35 µg/kg (considerably below the PNEC of 200 µg/kg).

2.1 Basic information

The analyses of first WL dataset are based on the data from 25 EU countries, with a total number of 35848 surface water samples in Sc2. The vast majority of these records are from river water samples (98.3%) but there are a few measurements for lakes (1.2%) and coastal/transitional water (0.5%). After the application of the PNEC quality criterion (explained in the chapter 2) the total amount of samples is reduced by 9.4% to 32482 records in Sc3.

Figure 1 shows in green colour the 25 countries which reported disaggregated data from the 1st year of WL monitoring (i.e. contributed to the WL dataset). The statistics per substance, about number of countries that reported measurements in all data scenarios, is shown in Annex 3. Only for information, for data in Sc1 one substance (methiocarb) did not pass the minimum representativity criterion for the number of countries with measurements.

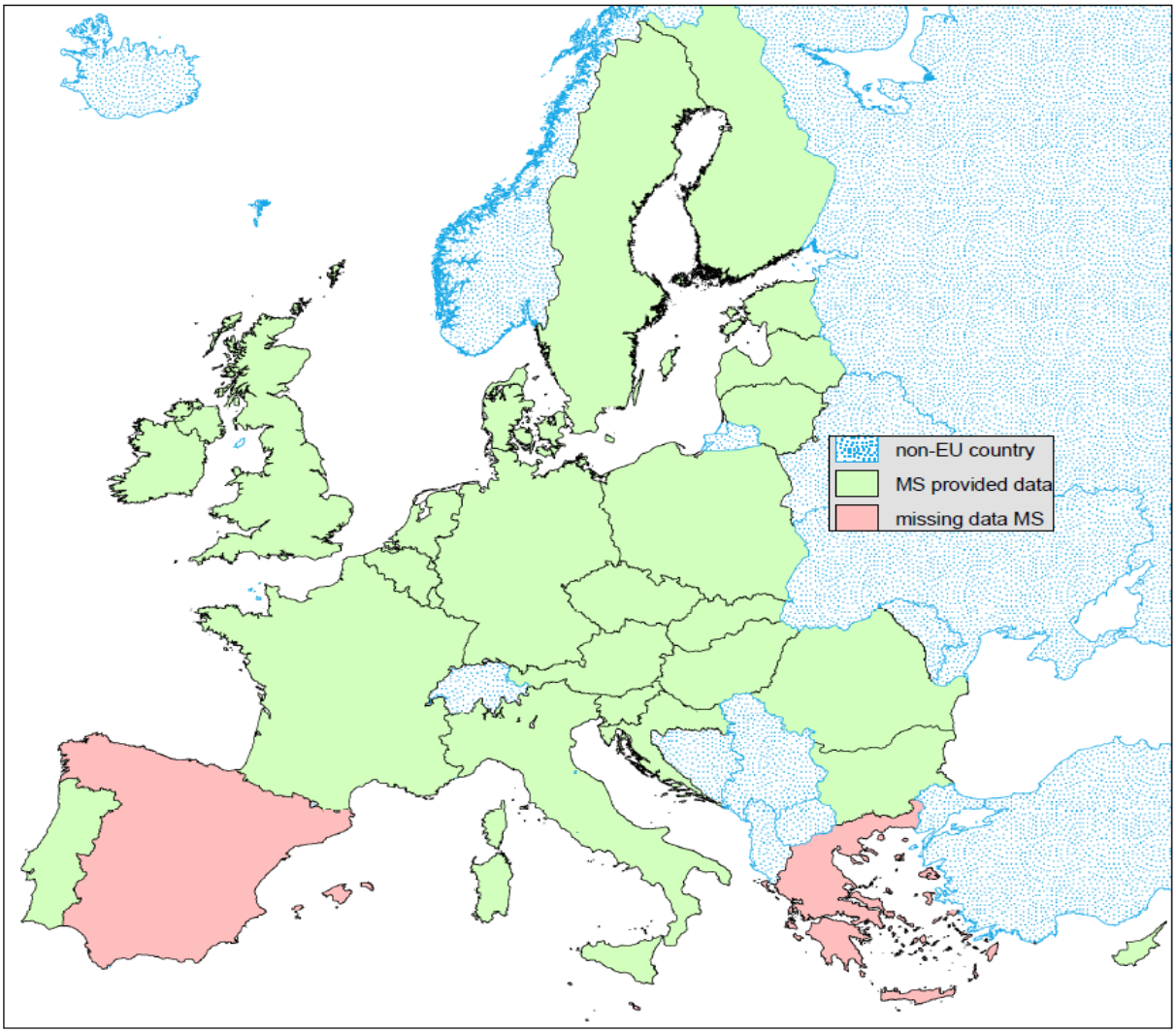


Figure 1: Map of countries having provided data for the first WL.

Conclusions:

Three MS did not report any disaggregated monitoring data for the first year of WL monitoring.

The analyses of first WL dataset are based on the data from 25 EU countries, with a total number of 35848 surface water samples for data in Sc2.

The vast majority of the sampling records in Sc2 of the WL dataset are from river water samples (98.3%).

There are a few measurements for lakes (1.2%) and coastal/transitional water (0.5%) in Sc2 of the WL dataset.

Insufficient sediment data were submitted for statistical analysis to be possible in Sc2 of the WL dataset.

2.2 Analysis by the number of sites

Figure 2 shows the number of monitoring sites (sampling stations) per substance for data of Sc2 (see details in Annex 3). Most of the substances were sampled at between 300

and 400 locations. The lower number of observation stations (201) is shown by 2-ethylhexyl-4-methoxycinnamate while diclofenac is the uppermost (608 sites). Thus, a sufficient number of sites for statistical analyses is available since when considering together the quantified and non-quantified samples for data in Sc2 all substances were measured at more than 200 sites.

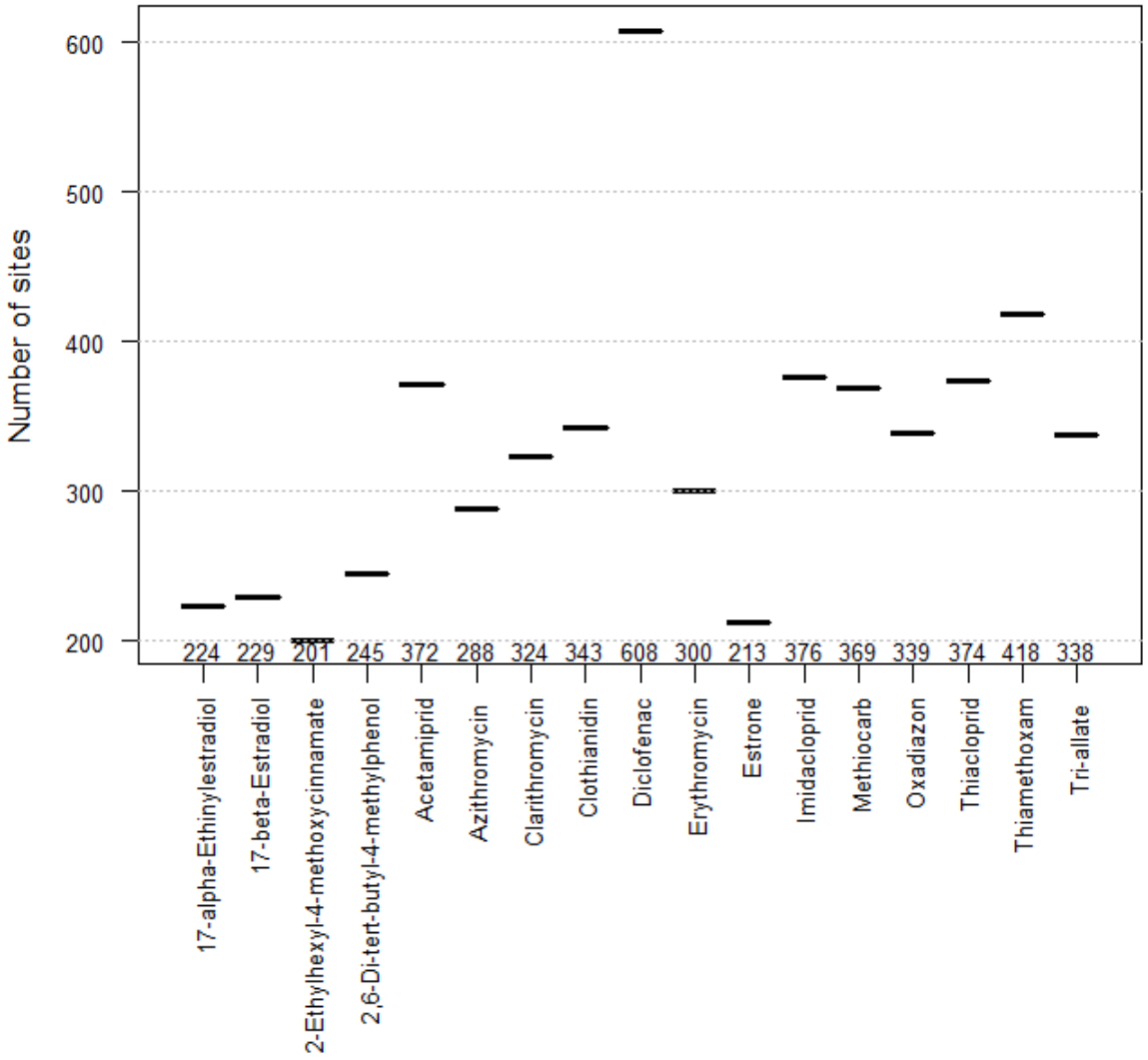


Figure 2: Number of monitoring sites per substance (Sc2).

Figure 3 displays the number of monitoring sites per country for dataset in Sc2 of the WL dataset. For most of the countries the number of monitoring sites has a range from 10 to 50. The country #21 has measured at smallest number of stations (2). The highest number of sites was reported by the country #06 (497) and the country #29 (53).

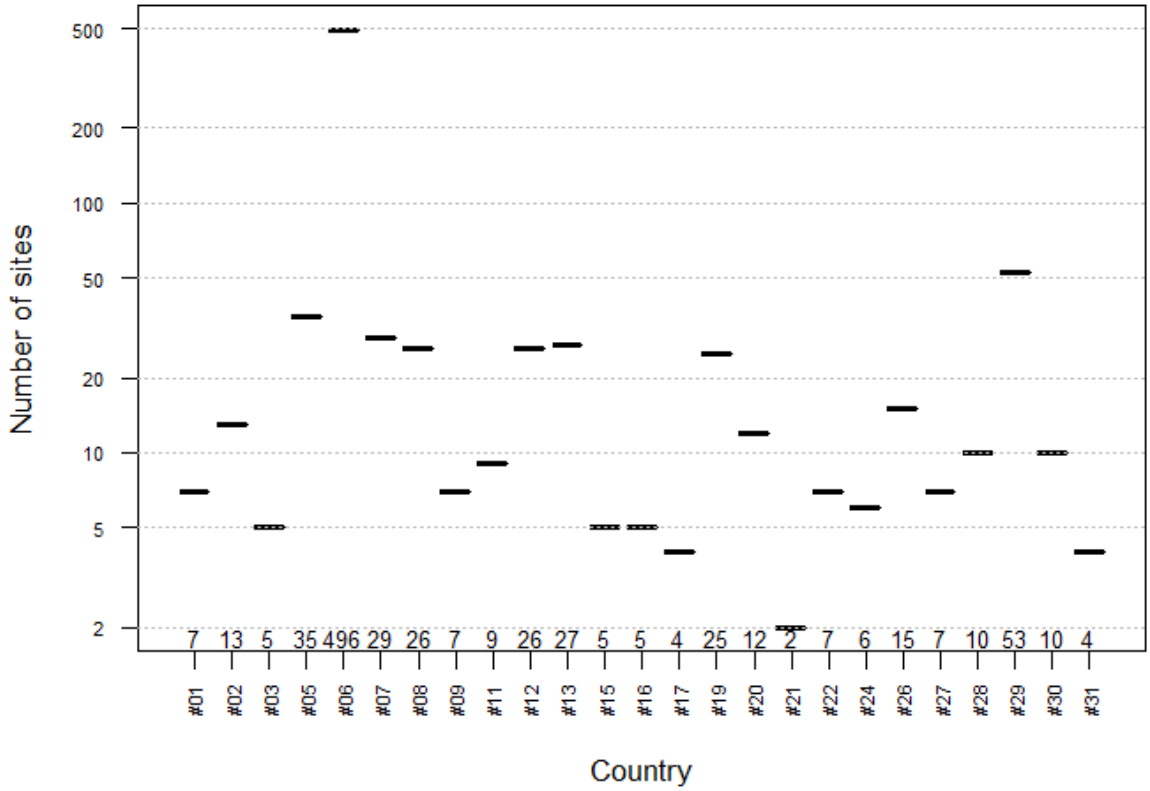


Figure 3: Number of sites (in logarithmic scale) per country (Sc2).

For monitoring data of Sc3, corresponding to the 2015 PNECs (see Annex 3.1) the statistical analysis of measurements for the WL substances evidenced that the lower number of monitoring sites is 123 (17-alpha-ethinylestradiol). For updated PNECs see details in Annex 3.2. Only for information, for data in Sc1 one substance (methiocarb) did not pass the minimum representativity threshold because it was quantified (or detected) above the LOQ only at 4 sites; in addition, acetamiprid was observed at the lower number of 10 sites.

Conclusions:

The reported monitoring data in Sc2 and Sc3 (corresponding to the 2015 PNECs) of the WL dataset contain a sufficient number of sites for statistical analyses since all substances were measured at more than 100 sites (Sc3). The analysis for Sc3 with the updated PNECs is presented in Annex 3.2.

2.3 Analysis by the number of samples

The total number of samples submitted up to the cut-off date (18 April 2017) was 35848 for surface water data of Sc2 (all monitoring records).

Figure 4 shows that for Sc2 the total number of samples per substance is ranging from 546 for 2-ethylhexyl-4-methoxycinnamate up to 6698 for diclofenac (see details in Annex 3). For most of the substances the range of the total number of samples is between 1000-3000.

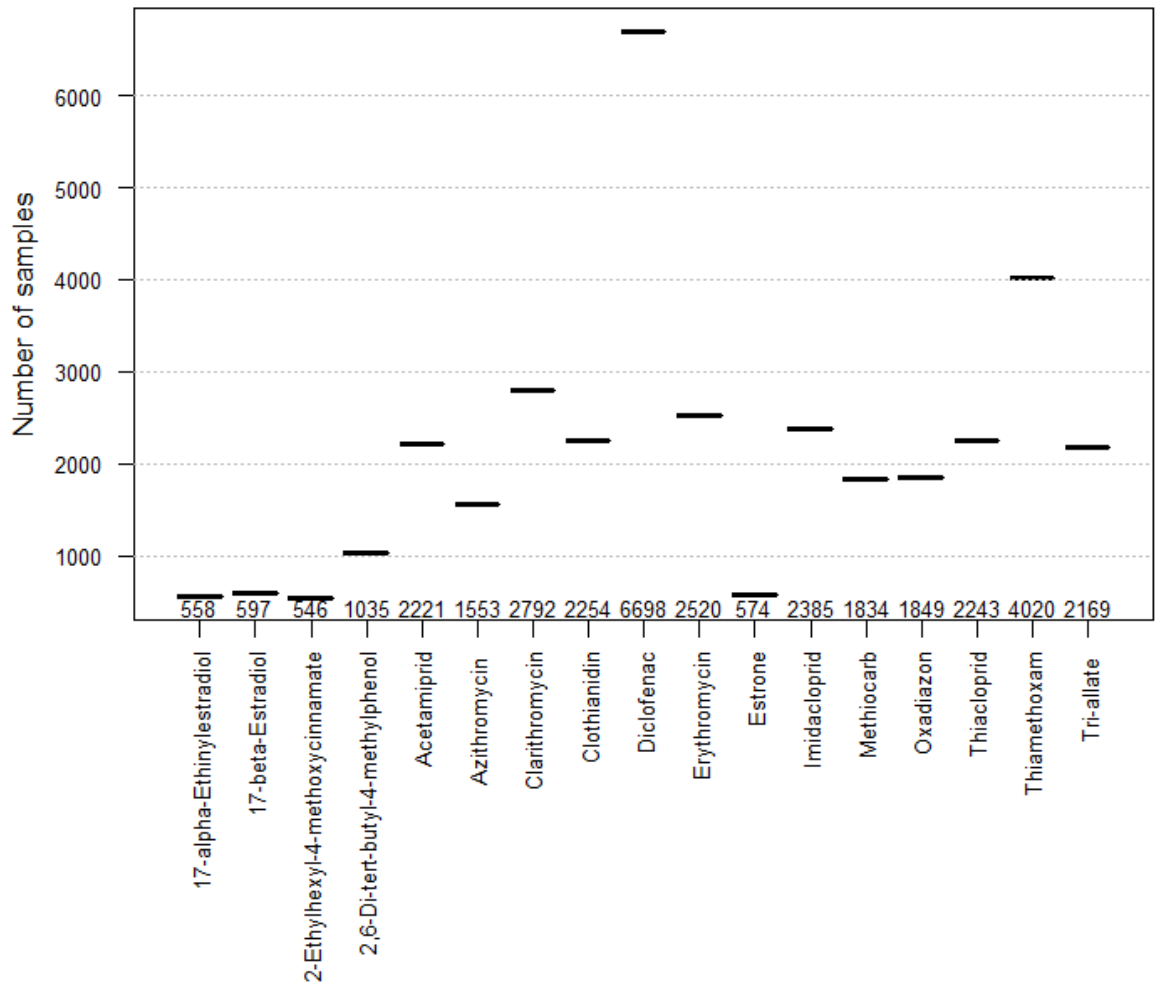


Figure 4: Number of samples per substance (Sc2).

For data of Sc3 (based on the 2015 PNECs) the statistical analysis (see Annex 3.1) showed that the lower number of monitoring samples is 226 (17-alpha-ethinylestradiol) and highest is 6698 (diclofenac). For updated PNECs see Annex 3.2. However, in Sc1 two substances have just a few samples (acetamiprid and methiocarb with 15 and 6 quantified samples, respectively) and among the other substances 2,6-di-tert-butyl-4-methylphenol was the lower observed with 57 quantified samples.

Figure 5 shows the total number of water samples per country for data of Sc2. Most of the countries have reported less than 1000 samples, with the exception of the countries #06 (25221; plus 582 samples for SPM and 290 for sediment), #07 (2279), #26 (2263), and #13 (1454). For the period 2014-2016 the amount of samples reported by one MS (#06) is about 70.4% of the total number of the collected samples. Seven countries (#15, #17, #20, #21, #22, #28, and #31) have reported less than 100 samples.

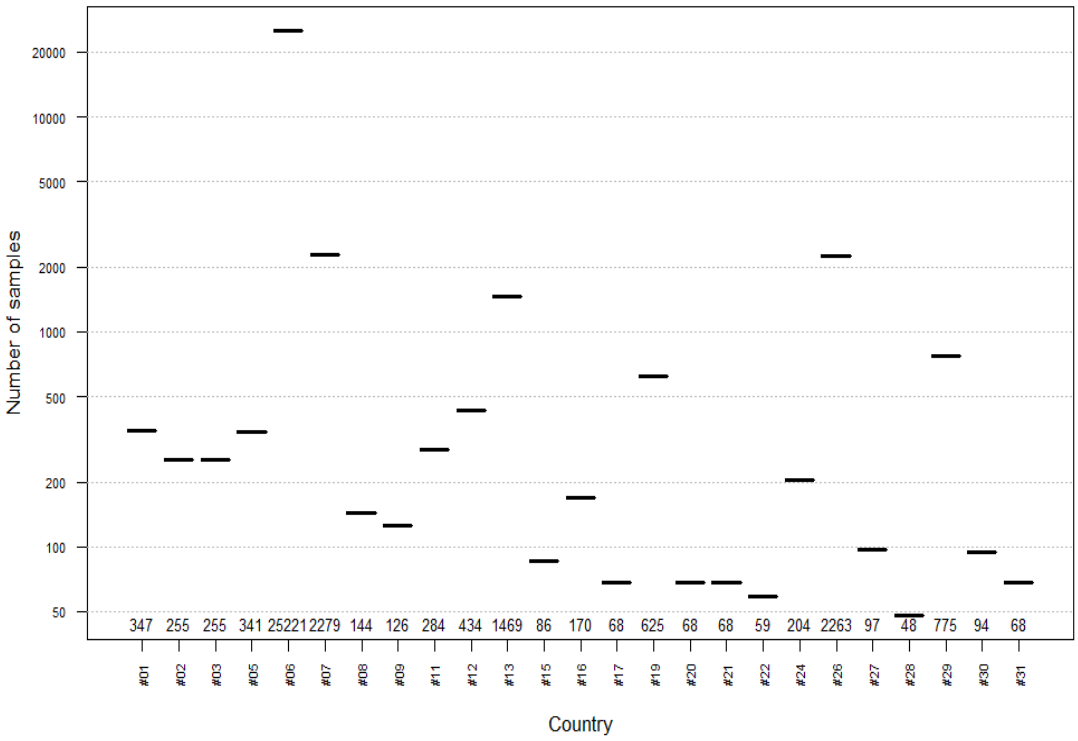


Figure 5: Number of samples (in logarithmic scale) per country (Sc2).

Figure 6 shows the number of samples per year for data of Sc2. Most of the samples reported are from the year 2016 (26056; 72.7% from the total number of samples), 6470 samples (18.1% from the total) are taken in the year 2015, and 3322 samples (9.2% from the total) are from the year 2014.

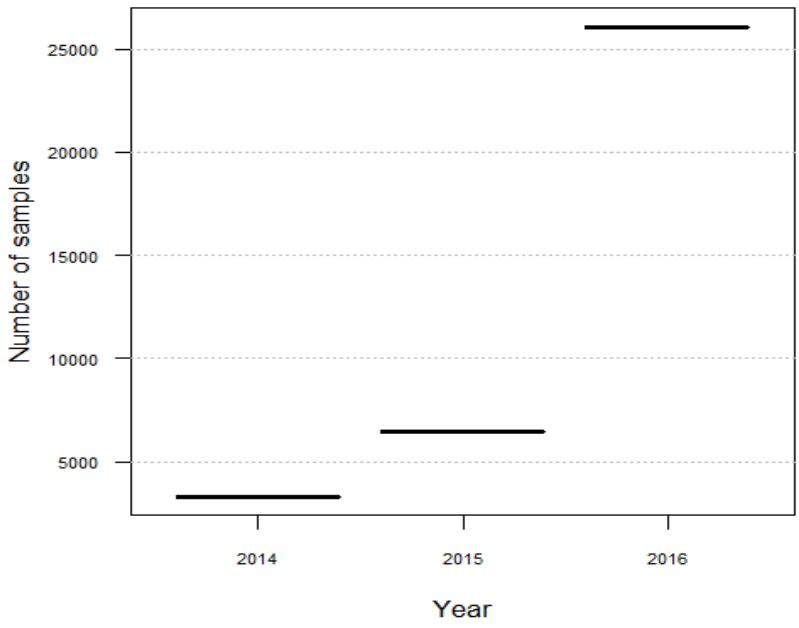


Figure 6: Number of samples per year (Sc2).

Figure 7 shows the number of samples per month and gives an idea about seasonality of the monitoring for data of Sc2 (on the figure January is indicated as 1, February by 2, etc.). In fact, most of the samples were taken between February and November. The peak of sampling is observed in the months of May and June.

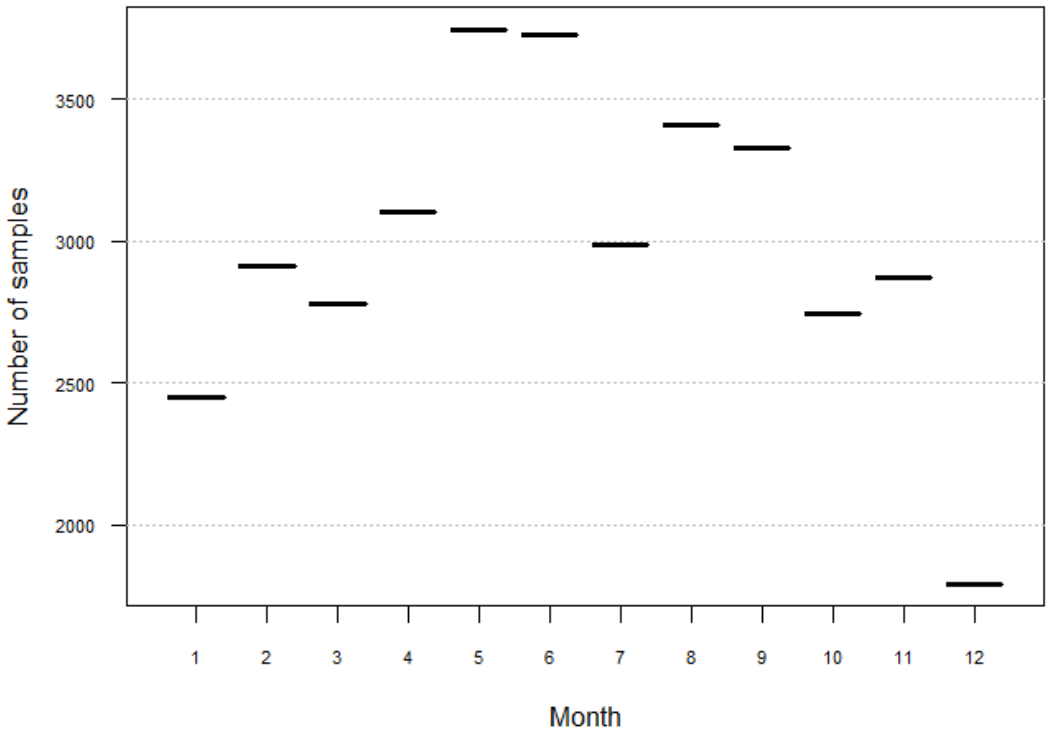


Figure 7: Number of samples per month (Sc2; January is indicated as 1, February by 2, etc.).

Conclusions:

In Sc2 and Sc3 (based on 2015 PNECs) all substances showed a sufficient amount of samples for statistical analyses since in Sc3 the minimum number of monitoring samples is 226 (17-alpha-ethinylestradiol). The analysis for Sc3 with the updated PNECs is presented in Annex 3.2.

The peak of WL sampling is observed in the months of May and June.

3. Additional analysis of WL dataset

3.1 Number of measured substances per country

Figure 8 shows the number of measured substances per country (Sc2). Nearly all countries reported measurements for all 17 substances of the first WL. The country #27 did not measure estrone (E1), and country #28 measured only 17-alpha-ethinylestradiol, 17-beta-estradiol and diclofenac.

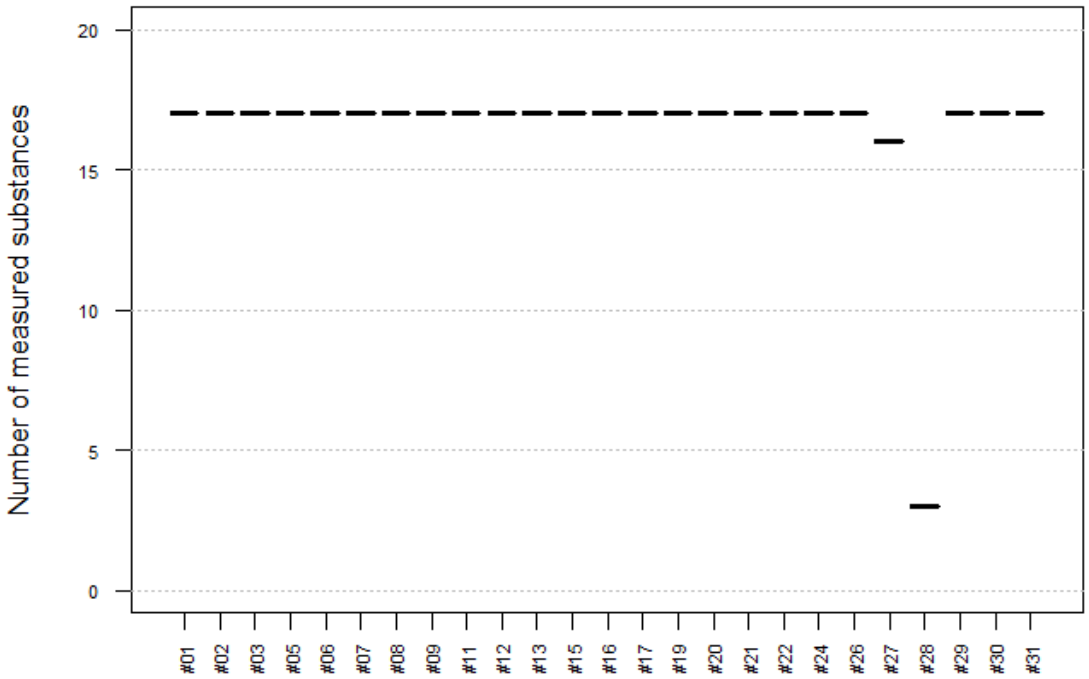


Figure 8: Number of measured substances per country (Sc2).

3.2 Months with measurements in each country

Figure 9 shows the months with measurements in each country of Sc2. For example, MS #01 has measured in all months from April to December (i.e. 9 months). The total number of months with sampling per country is indicated at the lowermost line of the figure. One MS (#17) reported samples only for one month. Several MS measured in two (#09, #12, #16, and #27), three (#03, #20, and #24) or four (#08, #11, #21, #30 and #31) months. Five MS (#02, #06, #07, #13, and #19) monitored in 11 or 12 months. This may not necessarily reflect that all WL substances have been measured in that frequency in a given country.

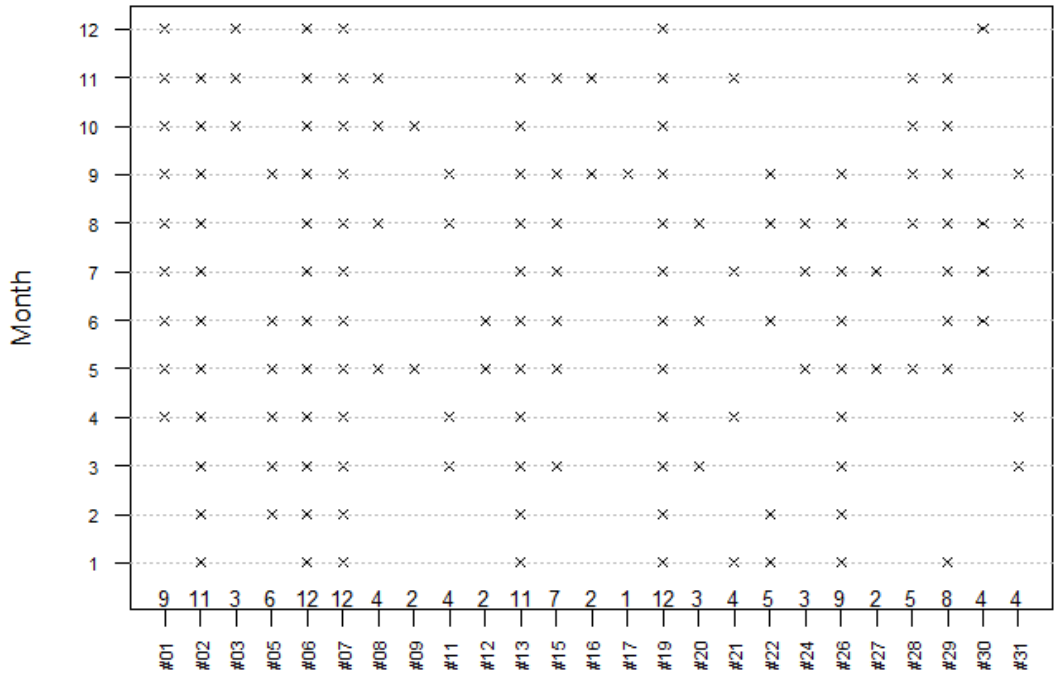


Figure 9: Months with measurements per country (Sc2; January is indicated as 1, February by 2, etc.). The total number of months with sampling per country is indicated at the lowermost line of the figure.

3.3 Ratio of number of samples and amount of sampling sites

Figure 10 shows per substance the ratio between the total number of samples and the total number of sampling sites for data in Sc2. For all substances the ratio is higher than 2 (maximum equals to 11) showing on average a sufficient frequency of sampling per site which supports the applicability of the STE method (in particular the Temporal factor).

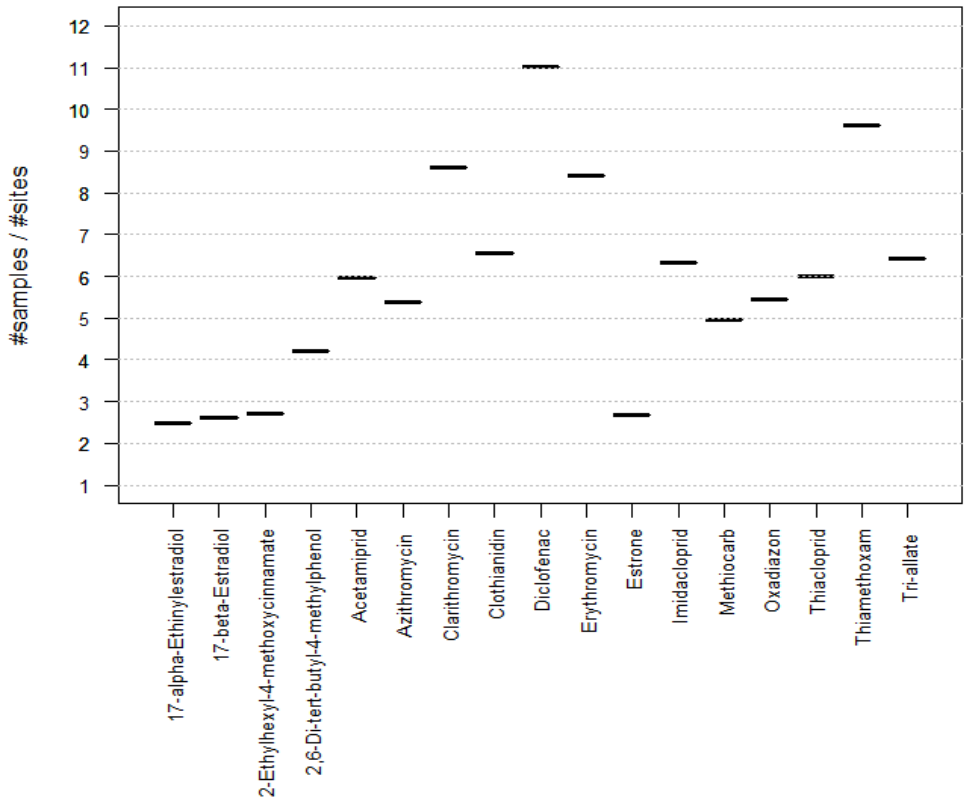


Figure 10: Ratio of number of samples and amount of sampling sites (Sc2).

3.4 Nearby pressure information

Article 8b of Directive 2013/39/EC states that "Member States shall monitor each substance in the watch list at selected representative monitoring stations over at least a 12-month period. In selecting the representative monitoring stations, the monitoring frequency and timing for each substance, Member States shall take into account the use patterns and possible occurrence of the substance. The frequency of monitoring shall be no less than once per year."

Accordingly, the MS have selected the monitoring stations representative of agricultural, urban, industrial pressures or a combination of these 3 types (and in addition in some cases "bathing water" for the sunscreen ingredient). However, only 12 MS reported the pressure information for the WL monitoring stations.

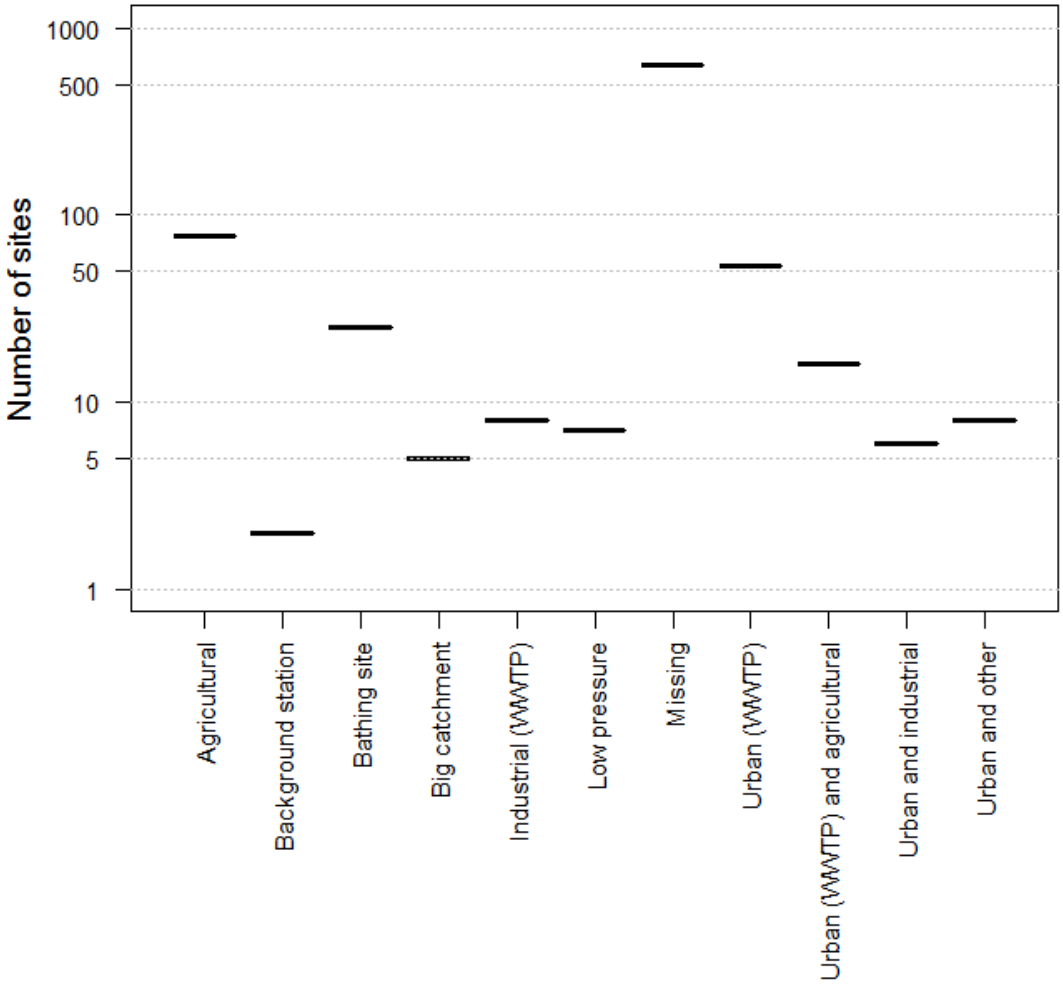
Some MS have provided additional information on the representativity of the monitoring stations and monitoring strategy. One MS stated for example: "The monitoring sites are selected in the vicinity of nearby pressures, but outside mixing zones and therefore the monitoring data reflect pressures realistically". Another MS stressed: "The selected monitoring stations are affected by either agricultural runoff or discharge from municipal wastewater treatment plants (MWTP) or by both". However, some MS have selected monitoring stations with low pressures (e.g. "at the end of the main rivers / catchment areas" (#28), or in big catchments) which are obviously not expected to show exceedances. Only one MS provided in their sampling strategy detailed information on the timing of sample collection.

Figure 11 displays the number of monitoring sites and the amount of samples under different types of relevant anthropogenic nearby pressures for data of Sc2. Unfortunately, for most of the sites (75.3%) and samples (79.3%) this information was not reported by MS. However, since a huge part of them (for instance 88.8% of the total

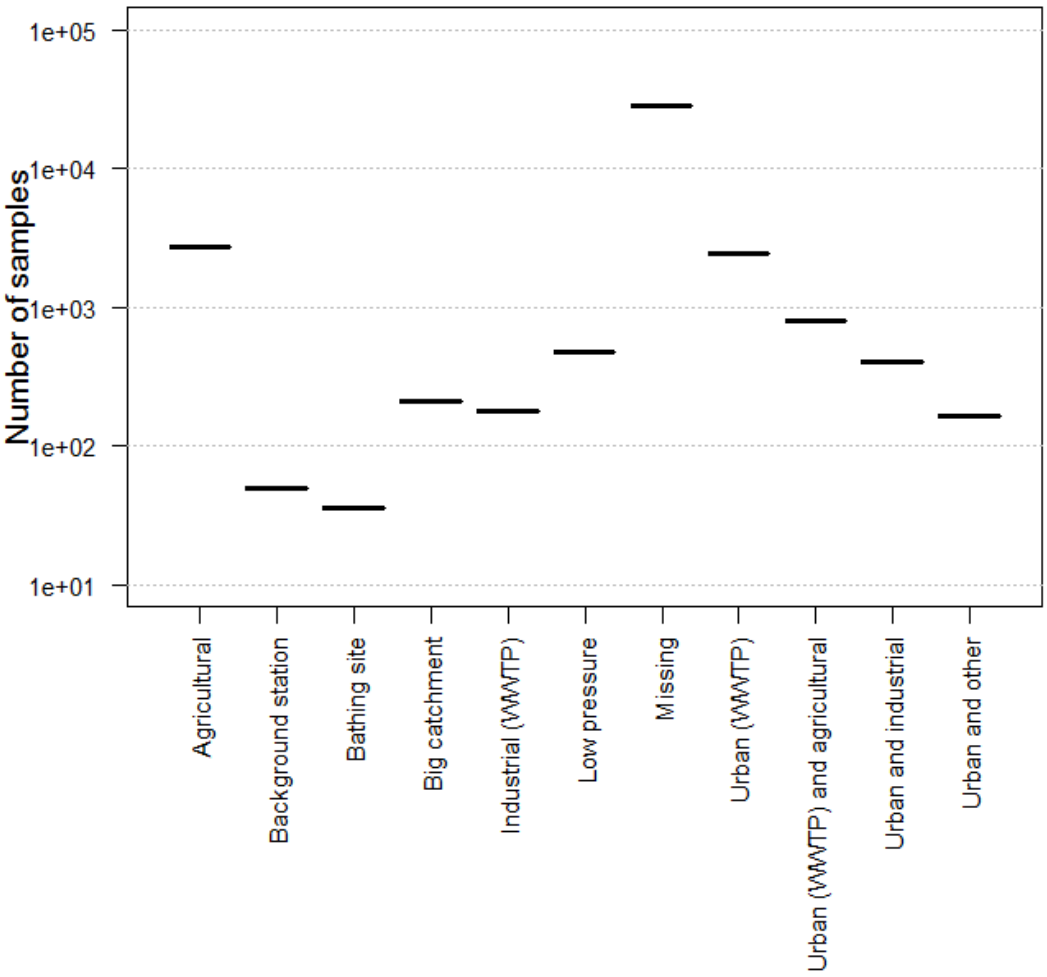
number of samples that missing pressure information) is from one MS (#06) this allows to making a relevant EU assessment. Most of the reported nearby pressures are defined as "agricultural" or "urban with WWTP impact".

For instance, considering the sunscreen ingredient 2-ethylhexyl-4-methoxycinnamate only 3 MS (#08, #22, and #29; all 3 are northern countries) have given the nearby pressure information "bathing site" for a total of 28 samples, which makes a correct data interpretation difficult.

The detailed graphical information (box-plots of concentrations) about the nearby pressures per substance is provided in Annex 7.1 (data in Sc3 and updated PNECs).



(a)



(b)

Figure 11: Number of monitoring sites (a) and the amount of samples (b) under different types of anthropogenic pressures (data in Sc2; the vertical axes are in Log scale).

Conclusions:

Two countries reported measurements not for all 17 substances of the first WL. The country #27 did not measure estrone (E1), and country #28 measured only 17-alpha-ethinylestradiol, 17-beta-estradiol and diclofenac.

For all substances the ratio between the total number of samples and the number of sampling sites is higher than 2 (maximum equals to 11) showing (on average) a sufficient frequency of sampling per site which supports the applicability of the Temporal factor of the STE method (Sc2).

For most of the sites (75 %) and samples (79 %) the anthropogenic nearby pressures were not reported by MS. However, since a huge part of them (for instance 88.8% of the total number of samples that missing pressure information) is from one MS (#06) that still allows to making a relevant EU assessment (Sc2).

In the first year of monitoring for the WL some MS have selected monitoring stations with low pressures (e.g. at the end of the main rivers / catchment areas or in big catchments) which are obviously not expected to show exceedances.

4 Data quality in WL dataset

Generally, the reporting and data quality in the first WL campaign is better compared to the quality of monitoring data collected in the last prioritisation exercise. As a result the processing of data has been faster and no outliers have been found in the first WL dataset.

4.1 Percentage of quantified samples

Figure 12 shows for Sc2 the percentage of quantified samples (measured concentration > LOQ) as a part from the total number of samples for the WL substances. For information the amount of these samples per substance is given at the lowermost line of the figure. Clarithromycin, diclofenac and estrone have a quantification frequency above 50%. Substances with a low quantification frequency (<10%) are listed in Table 4. Among them two substances (acetamiprid and methiocarb) have just a few quantified records and a very low percentage of quantification (below 1%).

All substances, except acetamiprid and methiocarb, have more than 51 quantified samples but 4 of them have less than 100 quantified measurements. Diclofenac and clarithromycin have a very high amount of quantified samples (4602 and 1642, respectively).

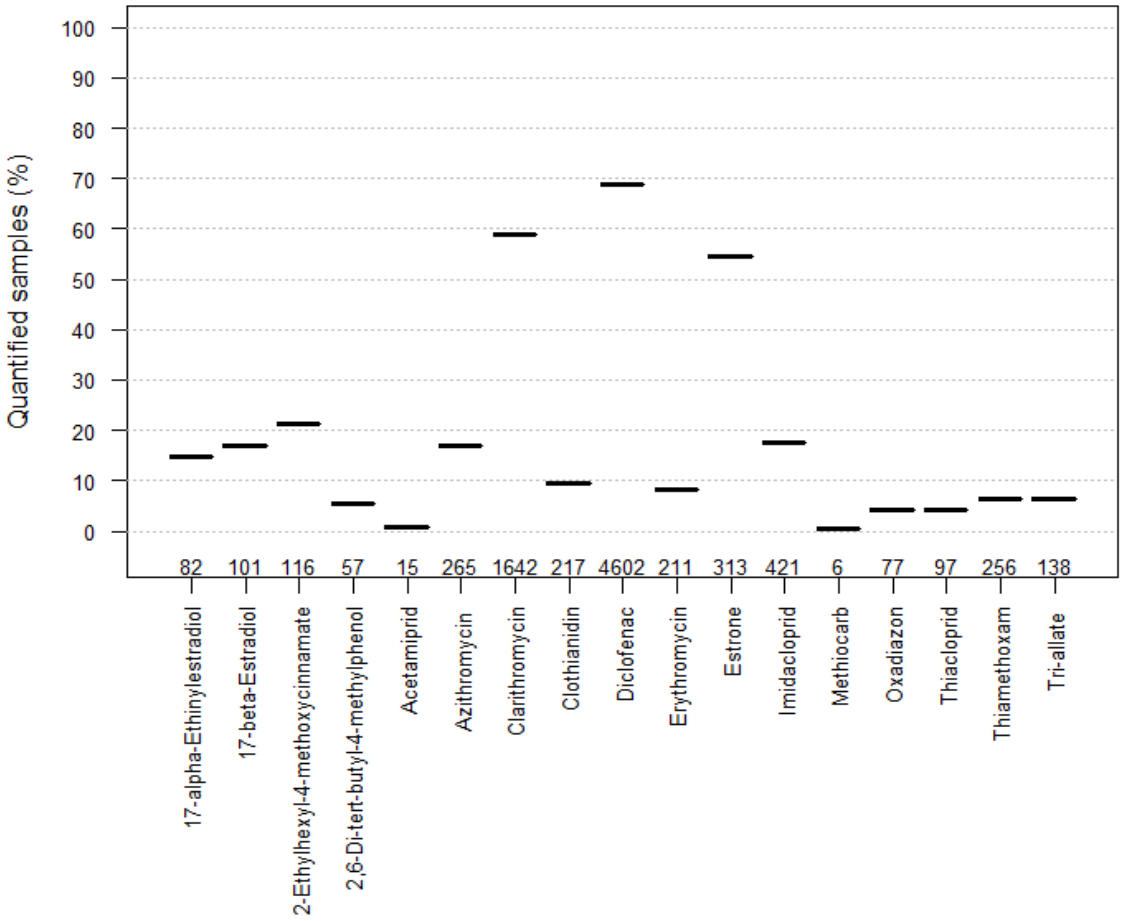


Figure 12: Percentage of quantified samples as a part from the total number of samples per substance (Sc2). The amount of quantified samples per substance is given at the lowermost line of the figure.

Table 4: Substances with quantification frequency (percentage of quantified samples from the total number of samples) below 10% (Sc2). Acetamiprid and methiocarb have just a few quantified records and a very low percentage of quantification (below 1%).

Substance	**Quantification frequency (%)** (the amount of quantified samples is given in brackets)
2,6-Di-tert-butyl-4-methylphenol	5.5 (57)
Acetamiprid	0.67 (15)
Methiocarb	0.33 (6)
Clothianidin	9.6 (217)
Erythromycin	8.4 (211)
Thiacloprid	4.3 (97)
Thiamethoxam	6.4 (256)
Oxadiazon	4.2 (77)
Triallate	6.4 (138)

4.2 Analysis of LOQs for the non-quantified samples

Firstly, Figure 13 compares per substance the range of LOQs (all countries together) with PNEC values from the WL report 2015 for the non-quantified samples in Sc2. The amount of non-quantified samples per substance is given at the lowermost line of the figure. It appears that for 17-alpha-ethinylestradiol (EE2) nearly all LOQs are above the PNEC of 0.000035 µg/L, indicating that it was very difficult for the laboratories to achieve the low PNEC of EE2. For 17-beta-estradiol (E2) around half of the LOQs are above the PNEC of 0.0004 µg/L. For estrone (E1), most of the LOQs are below the PNEC of 0.0036 µg/L. For imidacloprid (PNEC 0.009 µg/L) and methiocarb (PNEC 0.01 µg/L) around half of the LOQs are above the PNEC of these substances, showing that some MS had problems in achieving the PNEC values.

Thus, the first conclusion for data quality is that the results for the above-mentioned substances potentially have to be interpreted with care. All other substances were monitored by nearly all laboratories with analytical methods that "fit for purpose" (LOQ below PNEC).

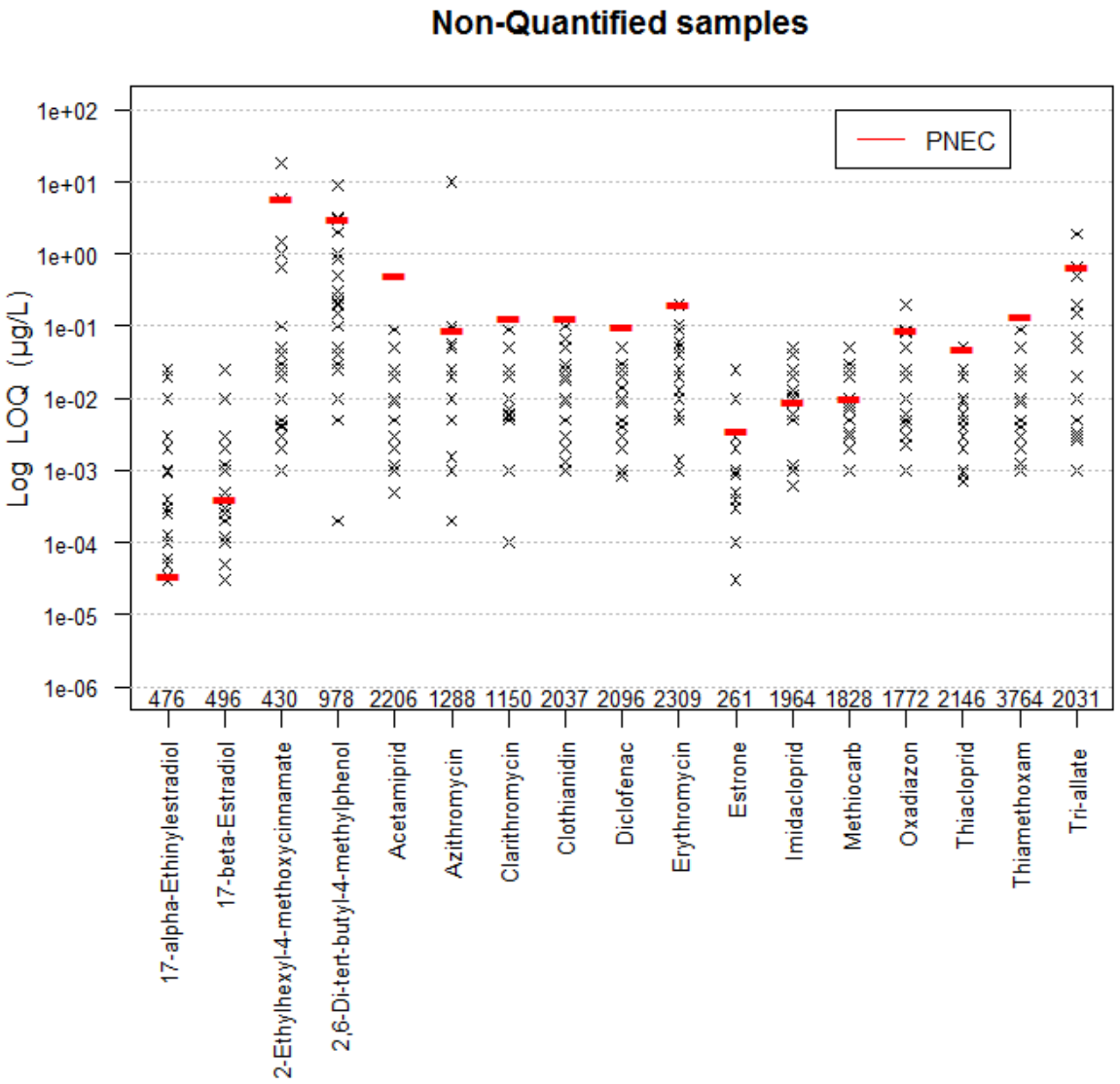


Figure 13: Range of LOQs for the non-quantified samples (in Sc2) per substance compared to PNEC values from the WL report 2015. The amount of non-quantified samples per substance is given at the lowermost line of the figure.

On the other hand, Figure 14 shows that for most of the WL substances in Sc2 data, the percentage of non-quantified samples with the 0.5*LOQ≤PNEC is more than 90%. The amount of these samples is given per each substance at the lowermost line of the figure. Indeed, only 3 substances that have very low PNECs showed relatively lower percentages of the non-quantified samples with 0.5*LOQ≤PNEC (17-alpha-ethinylestradiol with 50.6%; 17-beta-Estradiol with 72.8% and imidacloprid with 72.5%). Thus, for them an eventual difference between the STE scores for the different data scenarios could be anticipated. However, we could conclude, that although some problems in the analytical methods for 3 out of 17 substances exist (not sensitive enough to reach always PNEC), practically all substances have a sufficient number of samples with a good quality for making statistical analyses (the minimum is 241 samples for EE2).

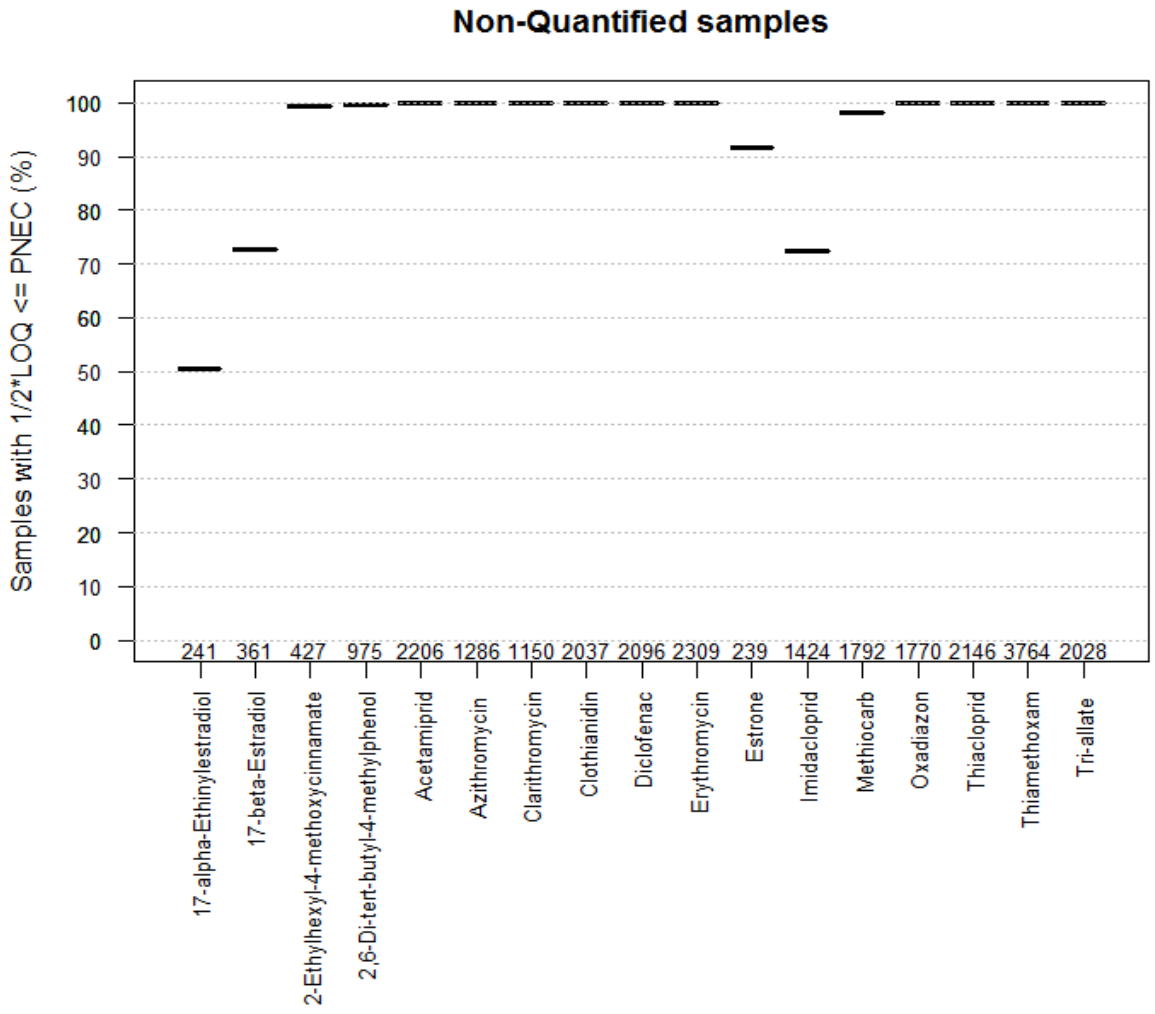


Figure 14: Percentage of non-quantified samples with 0.5*LOQ≤PNEC (in Sc2). The amount of these samples is given per each substance at the lowermost line of the figure. PNEC values correspond to the WL report 2015.

Additionally, for the WL substances with a reduced data quality a summary of the LOQ analysis regarding the achievement/non-achievement of PNEC value by country is presented below (for details see Annexes 4.1-4.5).

17-alpha-Ethinylestradiol (EE2)

A more detailed analysis of the LOQs for EE2 (non-quantified samples) showed that 4 MS achieved an LOQ of 0.03 ng/L (for 172 samples) which is below the PNEC (0.035 ng/L) (Annex 4.1). Other 4 countries reached an LOQ of 0.035 ng/L (for 57 samples), equal to the PNEC; 4 other countries have an LOQ of 0.1 ng/L (for 70 samples). There are however 12 countries with an LOQ clearly not sufficient for the low PNEC of 0.035 ng/L (for 247 samples).

17-beta-Estradiol (E2)

Annex 4.2 shows that for E2 most non-quantified samples have an LOQ ≤ the PNEC of 0.4 ng/L (360 out of 497 samples). The LOQs range from 0.03 – 25 ng/L. There are 16 countries which achieve with their analytical method the PNEC of E2, and 8 countries with higher LOQs.

Imidacloprid

Annex 4.4 shows the detailed analysis of the LOQs for imidacloprid (non-quantified samples); the LOQs range between 0.0006 - 0.05 µg/L. Most of the countries have reported for most of their samples an LOQ of 0.009 µg/l (123 samples in 8 countries) or 0.01 µg/l (1070 samples in 8 countries) which is equal (or nearly equal) to the proposed PNEC of 0.009 µg/L. There are however 11 laboratories (note that some MS report different LOQs from different laboratories) with 687 samples which do not achieve the PNEC.

Secondly, for Sc2 of WL dataset, Figure 15 shows a comparison of LOQs with the updated PNEC values while Figure 16 presents the percentage of non-quantified samples with 0.5*LOQ≤PNEC. The check of the WL dataset quality versus the updated PNECs showed that lower LOQs would be necessary also for azithromycin and methiocarb (imidacloprid is already flagged) to achieve these PNECs in addition to 3 substances identified for the PNECs of 2015.

Finally, we got an equivalent result when compared LOQs to the maximum acceptable method detection limit (according to Commission Implementing Decision EU/2015/495) as shown in Annex 4.6.

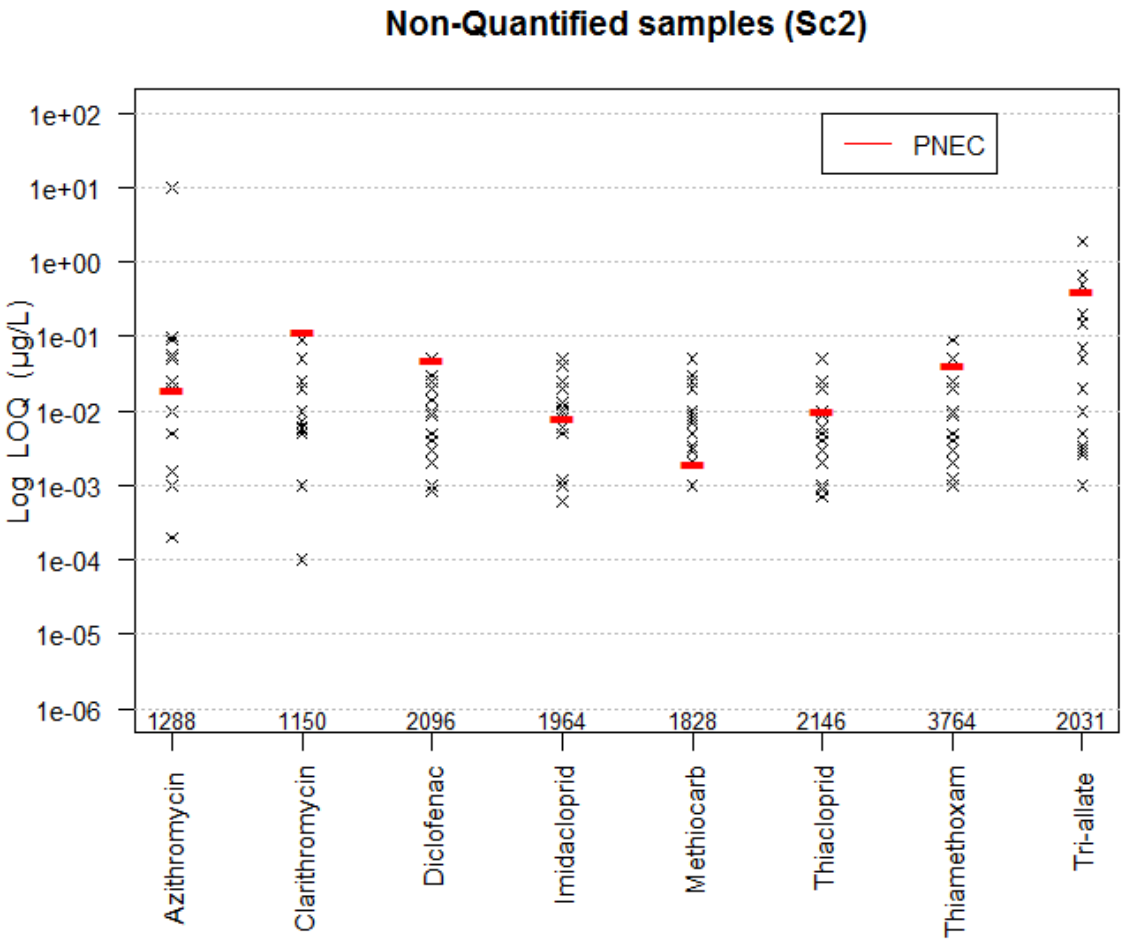


Figure 15: Range of LOQs for the non-quantified samples per substance compared to updated PNEC values (WL dataset in Sc2; only substances with the modified PNECs are shown). The amount of non-quantified samples per substance is given at the lowermost line of the figure.

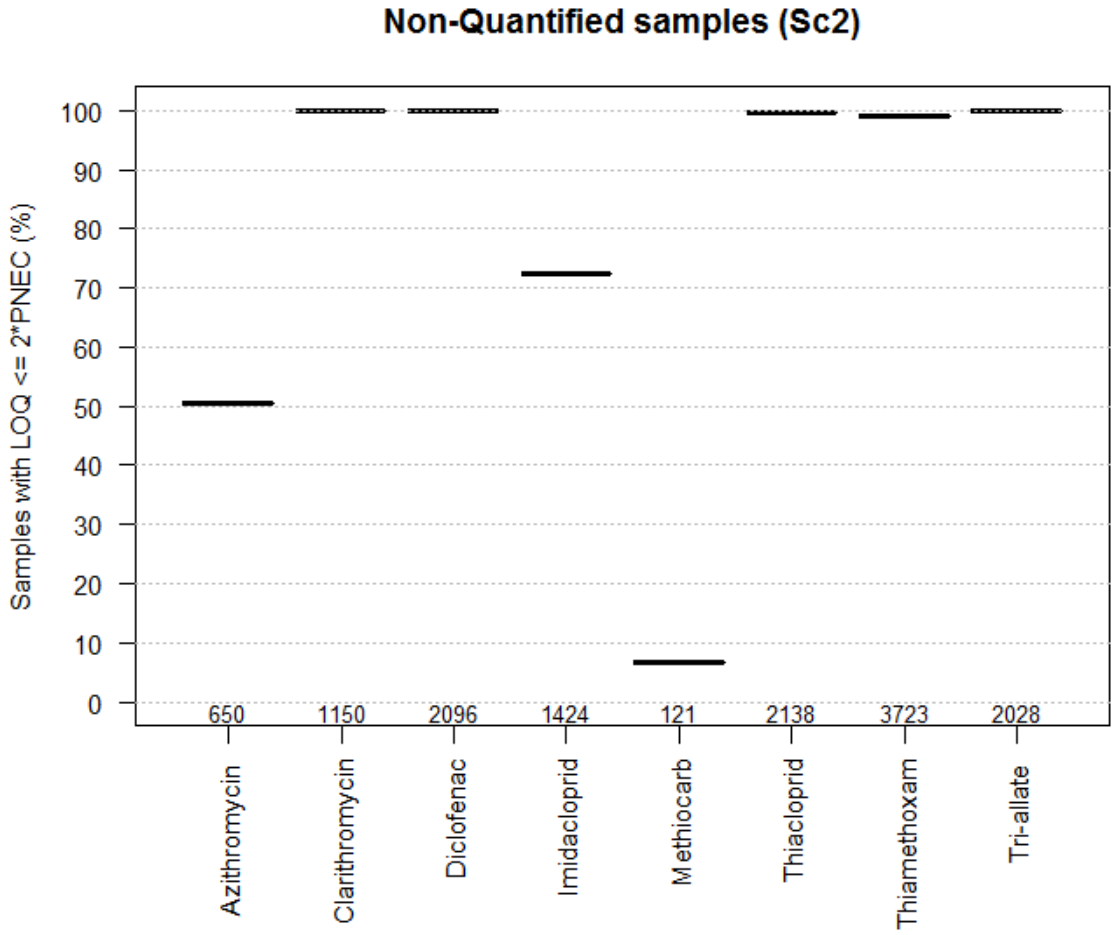


Figure 16: Percentage of non-quantified samples with 0.5*LOQ≤PNEC for WL dataset in Sc2 and updated PNECs (only substances with the modified PNECs are shown). The amount of these samples is given per each substance at the lowermost line of the figure.

4.3 Analytical methods

Exact methodological details (extraction volume; extraction method, clean-up; analytical instrument) on the analytical methods used for the analysis of the WL substances were provided by very few MS.

One MS (#22) which achieved the low PNEC of 0.000035 µg/l for EE2 has given the information to have extracted only 400 mL of water by liquid-liquid extraction and to have used a GC-MS-MS instrument of the latest generation (the derivatisation followed EPA Method 1698 (trimethylsilyl-ether) (Loos, 2015). In addition, country #26 has achieved for EE2 an LOQ of 0.00003 µg/l by the use of a SPE-GC-MS-MS method; no analytical details were however given.

Another MS (#19) which achieved the low PNEC of 0.000035 µg/l for EE2 has extracted 1 L of water by solid-phase extraction (SPE) with Oasis HLB cartridges followed by LC-MS-MS analysis.

It is therefore not totally clear why other MS could not reach the low PNEC of EE2. One possible solution to overcome the analytical difficulties for measuring E2, EE2 could be that MS which could not reach the PNEC values, could ask support to the MS having

successfully measured those substances. It would help to really understand if E2 and EE2 pose a risk at European level.

Conclusions (WL dataset and updated PNECs):

Nine out of 17 substances have a quantification frequency below 10 % for Sc2 and Sc3 (these substances are listed in Table 4). Among them acetamiprid and methiocarb have a very low quantification rate (less than 1%) and just a few quantified records.

Three substances (clarithromycin, diclofenac and estrone) have a detection frequency above 50% (for Sc2 and Sc3).

Practically all WL substances have in Sc3 and Sc2 a sufficient number of samples with good quality for making statistical analyses and STE applications, however, some MS had analytical problems to reach always the PNEC values for 5 out of 17 substances (EE2, E2, imidacloprid, azithromycin, and methiocarb).

One possible solution to overcome the analytical difficulties could be that MS that did not reach the PNEC values may ask support to the MS having successfully measured those substances. This would help to really understand if these substances pose a risk at European level.

5 Concentrations of WL substances by WL dataset

This section provides a summary-table of the monitored concentrations of WL substances in all data scenarios but visualises the concentrations by box-whisker plots only for Sc3 (PNECs either from the WL report 2015 or the updated ones). The detailed tabular statistics of the monitored concentrations of WL substances are given in Annex 3. In addition the information about the seasonal variability of WL substances and their concentrations per county is presented in Annex 7.2.

A box-whisker plot is a convenient way of graphically describing numerical data through their quartiles. The limits of the boxes represent the 25th and 75th percentiles while the line inside the each box specifies the median of the observed concentrations. Box-plots may also have lines extending vertically from the boxes (whiskers) indicating variability outside the upper and lower quartiles (spreading of data). The remote values are plotted as individual points.

5.1 PNECs from WL report 2015

Table 5 gives a summary of the concentration statistics for the WL substances and PNECs from WL report 2015.

It shows that the European median surface water concentration of EE2 is higher than the PNEC (0.035 ng/l) in the data scenarios Sc1 (0.1 ng/l) and Sc2 (0.05 ng/l); in Sc3 the median (0.015 ng/l) is lower than the PNEC.

The median concentration of diclofenac is between 0.027 µg/l (Sc3 and Sc2) and 0.047 µg/l (Sc1), of azithromycin 0.022 (Sc3 and Sc2) and 0.023 µg/l (Sc1), clarithromycin 0.016 (Sc3 and Sc2) and 0.034 µg/l (Sc1), and erythromycin 0.005 (Sc3 and Sc2) and 0.026 µg/l (Sc1).

The median concentration of imidacloprid exceeds its PNEC (0.009 µg/l) only in Sc1 (0.018 µg/l), but not in Sc2 (0.005 µg/l), or Sc3 (0.005 µg/l).

Figure 17 shows a box-whisker plot for the concentrations of the WL substances in Sc3 comparing to their PNEC values according the WL report 2015. The lowermost line of the figure indicates the total number of samples per substance.

The box-whisker plots for data of Sc2 and Sc1 are given in the Annex 3.1.

Table 5: Summary statistics of concentrations for the WL substances considering all data scenarios and PNECs (or EQS) from WL report 2015 (µg/l).

Substance	Scenario	Samples	PNEC	Median	Mean	P95	Max
	Sc1	82		**0.00010**	0.00023	0.00078	0.0030
17-alpha-Ethinylestradiol	Sc2	558	0.000035	**0.00005**	0.00055	0.0010	0.0125
	Sc3	323		0.000015	0.00007	0.00026	0.0030
	Sc1	101		0.00021	0.00041	0.00130	0.0030
	Sc2	597	0.0004	0.00017	0.00059	0.00150	0.0125
17-beta-Estradiol	Sc3	461		0.00015	0.00020	0.00051	0.0030
	Sc1	313		0.00064	0.0015	0.0050	0.031
	Sc2	574	0.0036	0.00050	0.0013	0.0050	0.031
Estrone	Sc3	552		0.00050	0.0010	0.0035	0.031
	Sc1	4602		0.047	0.093	0.34	2.6
	Sc2	6698	0.1	0.027	0.067	0.26	2.6
Diclofenac	Sc3	6697		0.027	0.067	0.26	2.6
	Sc1	57		0.018	0.512	0.26	14.0
2,6-Di-tert-butyl-4-methylphenol	Sc2	1035	3.16	0.0050	0.10	0.25	14.0
	Sc3	1032		0.0050	0.088	0.25	14.0
	Sc1	116		0.305	0.420	1.4	1.8
2-Ethylhexyl-4-methoxycinnamate	Sc2	546	6.0	0.050	0.367	3.0	9.0
	Sc3	543		0.050	0.319	3.0	3.0
	Sc1	211		0.026	0.060	0.20	1.1
	Sc2	2520	0.2	0.0050	0.012	0.028	1.1
Erythromycin	Sc3	2520		0.0050	0.012	0.028	1.1
	Sc1	1642		0.034	0.073	0.28	1.6
	Sc2	2792	0.13	0.016	0.047	0.17	1.6
Clarithromycin	Sc3	2792		0.016	0.047	0.17	1.6
	Sc1	265		0.023	0.062	0.25	1.0
	Sc2	1553	0.09	0.022	0.030	0.055	5.0
Azithromycin	Sc3	1551		0.022	0.023	0.053	1.0
	Sc1	6		0.028	0.040	0.090	0.109
	Sc2	1834	0.01	0.0050	0.0061	0.010	0.109
Methiocarb	Sc3	1798		0.0050	0.0059	0.010	0.109
	Sc1	421		**0.018**	0.031	0.082	1.05
	Sc2	2385	0.009	0.0050	0.011	0.027	1.05
Imidacloprid	Sc3	1830		0.0050	0.011	0.033	1.05
	Sc1	97		0.015	0.026	0.079	0.57
	Sc2	2243	0.05	0.0050	0.0068	0.010	0.57
Thiacloprid	Sc3	2243		0.0050	0.0068	0.010	0.57
	Sc1	256		0.015	0.032	0.123	0.77
	Sc2	4020	0.14	0.0050	0.0076	0.013	0.77
Thiamethoxam	Sc3	4020		0.0050	0.0076	0.013	0.77
	Sc1	217		0.016	0.044	0.173	0.78
	Sc2	2254	0.13	0.0050	0.011	0.033	0.78
Clothianidin	Sc3	2221		0.0050	0.011	0.033	0.78
	Sc1	15		0.0090	0.014	0.045	0.074
	Sc2	2221	0.5	0.0050	0.0067	0.010	0.074
Acetamiprid	Sc3	2221		0.0050	0.0067	0.010	0.074
	Sc1	77		0.010	0.023	0.071	0.31
	Sc2	1849	0.088	0.0050	0.011	0.040	0.31
Oxadiazon	Sc3	1847		0.0050	0.011	0.040	0.31
	Sc1	138		0.022	0.037	0.113	0.270
	Sc2	2169	0.67	0.0050	0.015	0.035	0.945
Triallate	Sc3	2166		0.0050	0.014	0.033	0.335

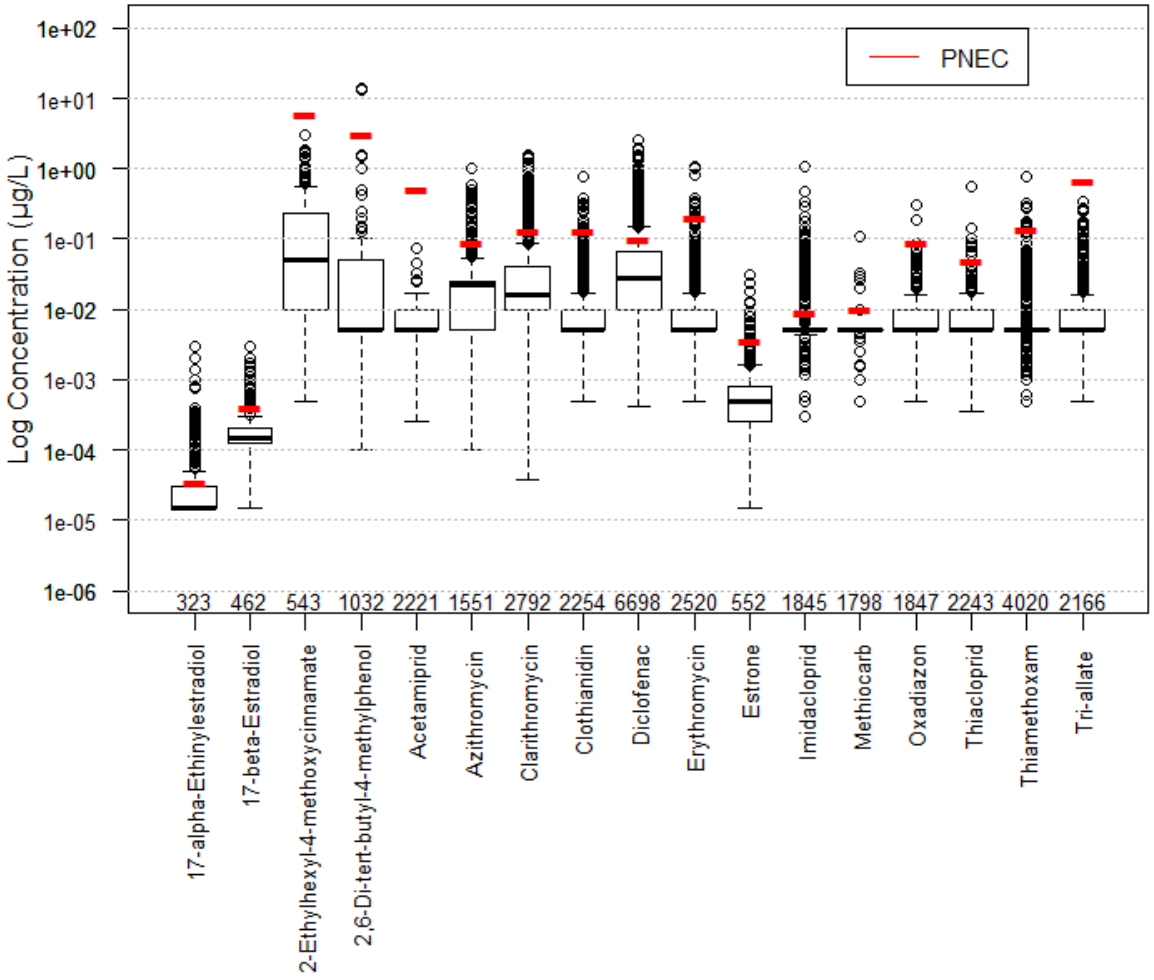


Figure 17: Box-plot of concentrations (log scale) for WL substances (Sc3) comparing to the PNEC values from the WL report 2015. The lowermost line of the figure indicates the total number of samples per substance.

5.2 Updated PNECs

Figure 18 shows a box-whisker plot for the concentrations of WL substances in samples of Sc3 in comparison to the updated PNEC values. The lowermost line of the figure indicates the total number of samples per substance. Attention should be paid on the changes for some substances (for instance the number of samples, PNECs, etc.) when applying the updated PNECs.

The box-whisker plots for data of Sc2 and Sc1 are given in the Annex3.2.

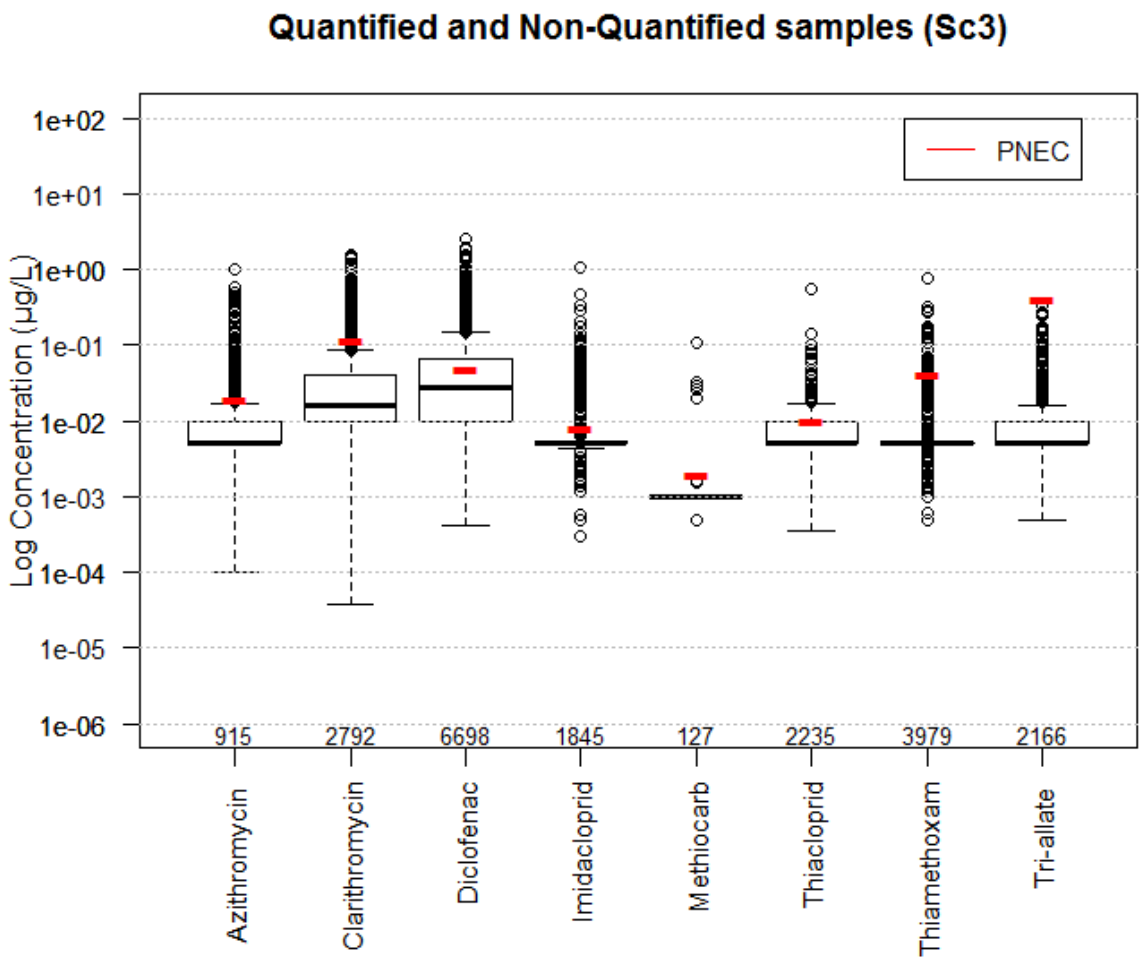


Figure 18: Box-plot of concentrations (log scale) for WL substances (Sc3) comparing to the updated PNEC values (only substances with the modified PNECs are shown). The lowermost line of the figure indicates the total number of samples per substance.

6 STE scores of WL substances by WL dataset

For the evaluation of the risk of the WL substances the STE assessment tool was run for monitoring data in all data scenarios (Sc1, Sc2 and Sc3) and diverse PNEC values (WL report 2015 and the updated PNECs). However, following the established practice of the sub-group on revision of the priority substances list, Sc3 is considered as the most relevant scenario for making assessments. The risk is quantified according to 5 levels of the STE scores as follows: very high 2.4-3; high 1.8-2.4; intermediate 1.2-1.8; low 0.6-1.2; very low 0.0-0.6)[11].

6.1 PNECs from 2015

The tabular comparison of STE scores calculated by the three data scenarios is presented in Annex 5.1 together with the additional specific information about the individual STE factors in scenario Sc3.

Figure 19 presents the STE scores for Sc3 and Sc2 with the PNECs from the WL report 2015. All scores in Sc3 are below 1. The Sc2 leads usually to higher STE results. This is explained by the assignment in Sc2 of the artificial concentrations of ½ LOQ to all non-quantified values, while part of these values are excluded from Sc3 (after the application of the PNEC quality criterion) if the analytical method is not able to detect the substance close to its PNEC. The biggest deviation between the scores for Sc3 and Sc2 was found mostly for substances that were already identified having a reduced data quality (see section 5). Expectedly, the results for Sc1 are higher comparing to the other two scenarios (Sc1 is not shown in the figure; see details in Annex 5.1).

[11] This cut-off threshold was used to reach a list of substances showing very high and high risk score, however it doesn't mean that substances with intermediate STE score may not pose a risk at EU-level.

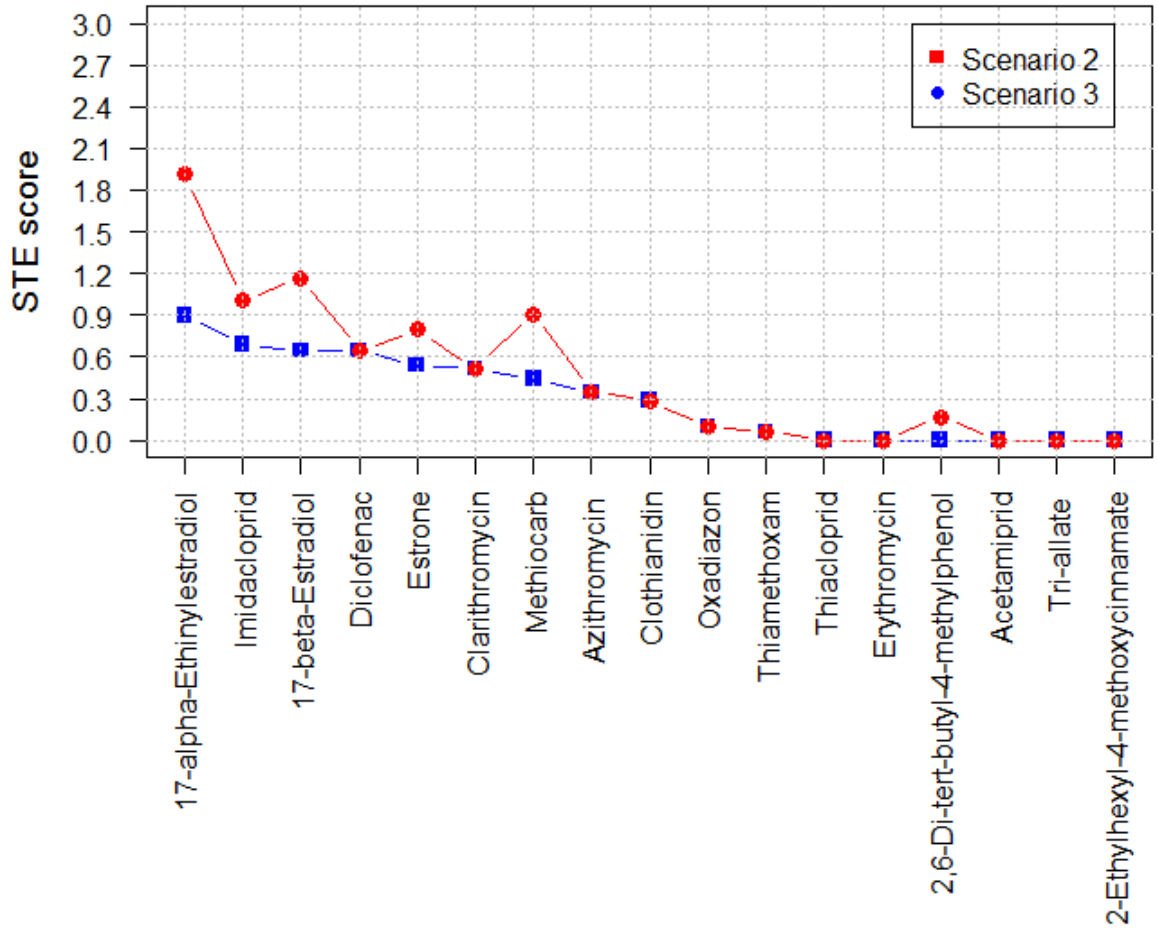


Figure 19: Comparison of STE scores obtained for Sc2 and Sc3 of WL dataset (PNECs from WL report 2015).

6.2 Updated PNECs

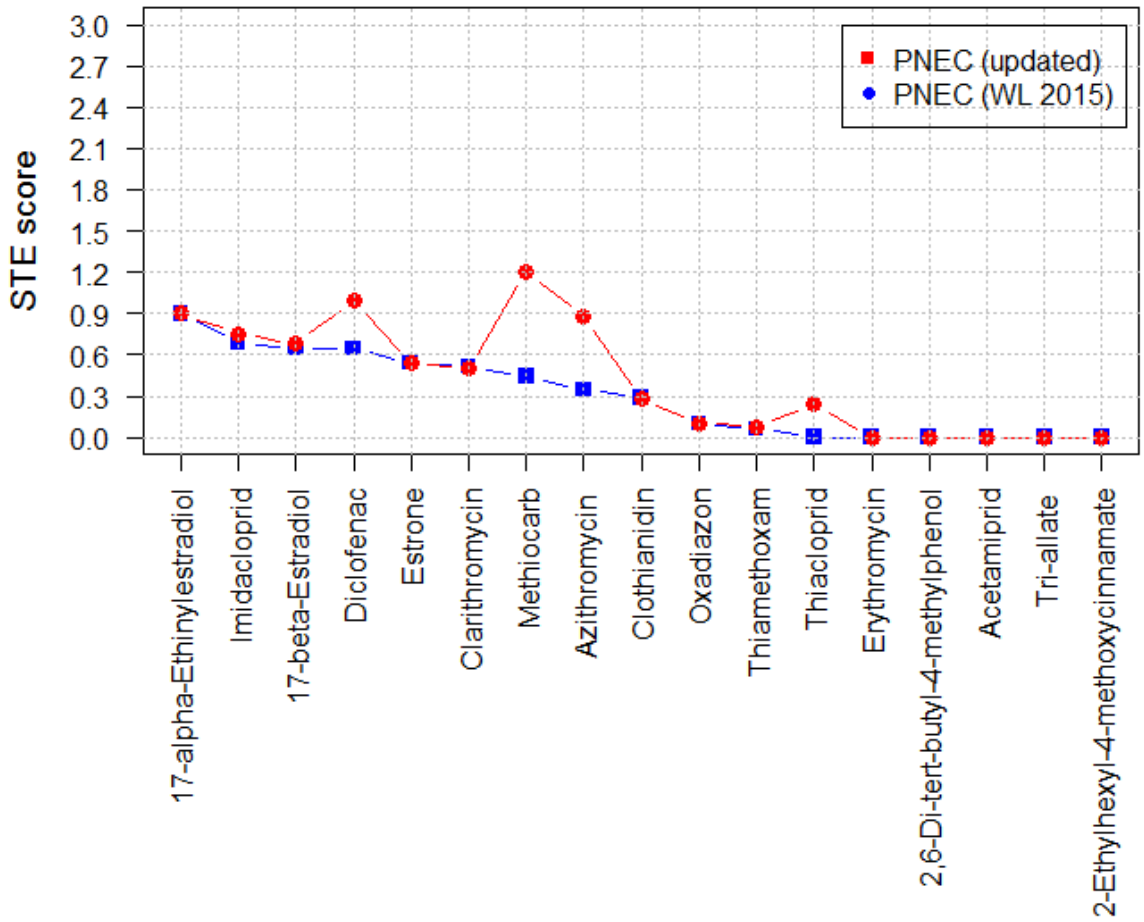


Figure 20 shows, on average, a small to medium increase of STE scores for diclofenac, azithromycin and thiacloprid after the application of the updated PNECs to the WL monitoring data in Sc3. The details for the scoring in all data scenarios and updated PNECs could be followed in Annex 5.2 in a tabular form.

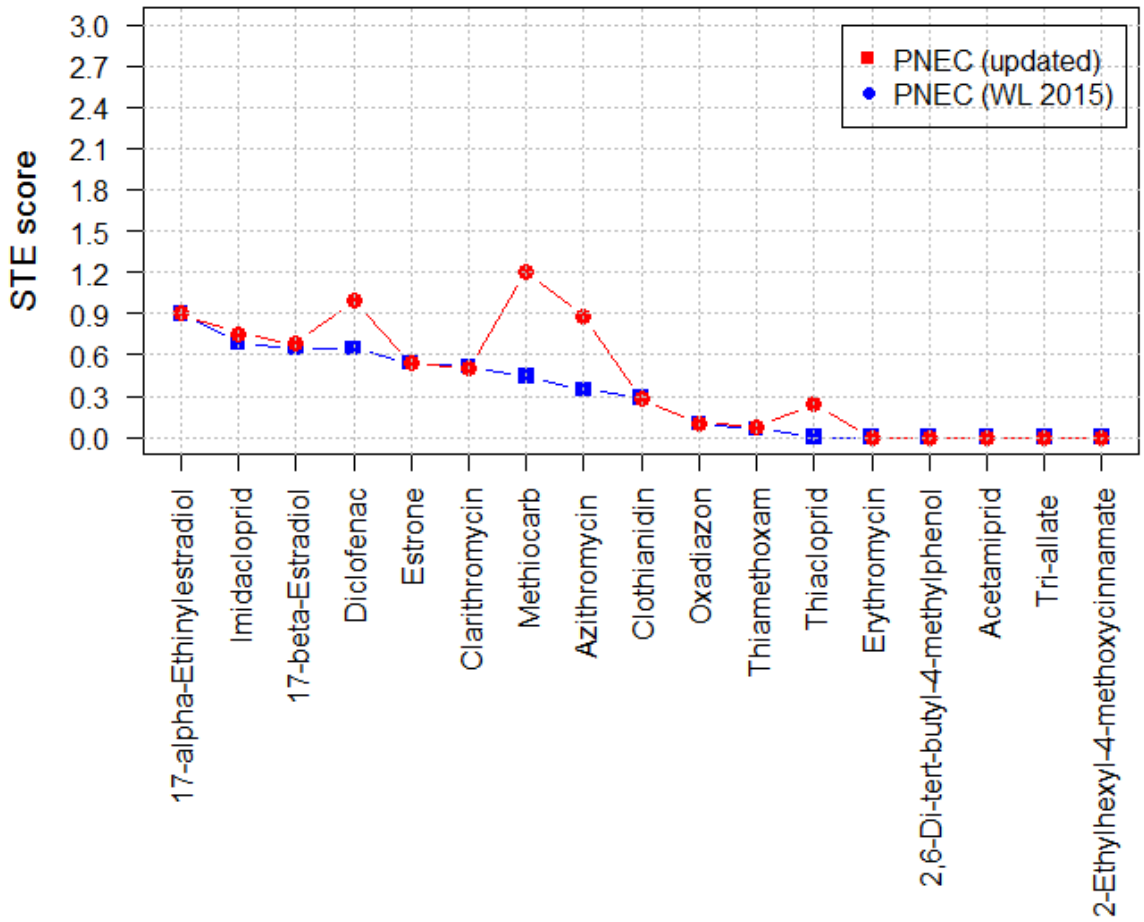


Figure 20: Comparison of STE scores obtained using WL dataset in Sc3 scenario for different PNEC values (from WL report 2015 and updated ones).

Conclusions:

For the PNEC values from the WL report 2015, the STE scores in Sc3 are below 1 for all WL substances. The usage of data in Sc2 leads usually to higher STE results. The biggest deviation between the scores in Sc3 and Sc2 was found mostly for substances that were identified having a reduced data quality.

There is on average, a small to medium increase of STE scores for diclofenac, methiocarb, azithromycin and thiacloprid after the application of the updated PNECs (WL dataset in Sc3).

7 Discussion

7.1 Review of the 1st WL

This section first proposes a set of criteria to determine whether there is enough, high-quality EU-wide monitoring data to assess the risk posed by each WL substance. On this basis, a list of substances that can be taken out of the WL is then identified.

7.1.1 Criteria for the removal of substances from the WL

The EQS Directive states: "The Commission shall establish the first watch list by 14 September 2014 and shall update it every 24 months thereafter. When updating the watch list, the Commission shall remove any substance for which a risk-based assessment as referred to in Article 16(2) of Directive 2000/60/EC can be concluded without additional monitoring data."

Respecting the requirements of the EQS Directive, the removal of the substances from the WL is determined by the high data quality which is defined by the following criteria (proposed by the JRC) and both of them have to be fulfilled:

1. The ½ LOQ must be below or equal to the PNEC, for at least 90 % of the non-quantified samples in Sc2 (LOQ-PNEC criterion).
2. Similarity of STE scores for Sc3 and Sc2 (no more than 15 % difference in STE scores demonstrating no significant analytical problem with non-quantified samples).

Note: the difference of the STE scores is calculated as a percentage by the formula $|STE_{Sc3} - STE_{Sc2}| / STE_{Sc3} * 100$

Rationale behind the criteria:

Criteria 1: As mentioned in the summary and in the introduction, scenario 3, which gathers non quantified samples with LOQ/2≤PNEC and quantified samples, is considered to be the most relevant scenario to assess the risk and to calculate the STE score. Criteria 1 ensures that most of the samples in scenario 2 (i.e. in the full dataset) are of sufficient quality to be included in scenario 3, and thus to assess the risk posed by the substance calculating its STE score.

Criteria 2: Sc2 differs from Sc3 because Sc2 includes non-quantified samples for which LOQ/2>PNEC. As explained previously, these non-quantified samples are replaced by LOQ/2 in the calculation of the STE score thus leading to non-confirmed exceedances (concentrations above the PNEC). If the STE scores are similar in Sc2 and Sc3, this means that the non-quantified samples with a high LOQ (LOQ/2>PNEC), and the related "non-confirmed exceedances", have a relatively limited impact on the risk assessment/STE score for the substance. In other words, the datasets of Sc2 and Sc3 have to be similar. This indicates overall reliability in the assessment based on the monitoring data.

7.1.2 Implementation of the removal criteria on the WL dataset

As explained earlier, the above criteria were implemented on the WL dataset with the updated PNEC values (see details in Table 7). We found that 10 substances fulfil both criteria simultaneously: diclofenac, clarithromycin, erythromycin, oxadiazon, tri-allate,

2,6-di-tert-butyl-4-methylphenol, acetamiprid, clothianidin, thiacloprid, and 2-ethylhexyl-4-methoxycinnamate.[12]

These results are confirmed when using the combined dataset and the updated PNEC (see details in Annex 6.2). The only difference lies in the fact that thiacloprid does not fulfil the above criteria when using the combined dataset, thus pointing to a lower quality of the combined dataset for this substance[13].

However to come to the final list of substances to be removed from the WL it should be noted and taken into account that:

- Neonicotinoids and macrolide antibiotics were included as groups in the WL, and all substances in each of these groups can be monitored with the same analytical method, so it makes sense to keep them jointly in the WL. In addition, ongoing work at EU-level[14] may lead to a change in the conditions of approval of several of the neonicotinoids, thus possibly leading to substitution effects, and to changes in the risk posed by these substances. Consequently, the data collected so far under the WL may possibly not reflect the risk posed by the substances in the very near future, and it makes sense to keep them in the list to gather sufficient, high quality monitoring data to confirm the risk they pose.

- As regards the sunscreen ingredient 2-ethylhexyl-4-methoxycinnamate, it is unclear how far the monitoring sites selected were representative of the relevant pressure (samples should be taken preferentially in the summer at bathing sites). Consequently more monitoring data, at the relevant sites and in the relevant period need to be gathered before its removal from the list can be confirmed. It is also worth noting that this substance was initially recommended for monitoring in sediment[15], but that most data received were for water. The few sediment data reported to the JRC were not enough to carry out a conclusive analysis for that matrix. Consideration is being given to include several substances for sediment monitoring in a WL update in 2019. Therefore we propose the removal of the sunscreen ingredient (currently monitored in water) from the current WL in 2018, and its reinclusion in 2019 for monitoring in sediment together with the other candidate substances mentioned below. This will ensure the timely and cost-efficient development / validation of analytical methods (in particular by optimising the use of sediment samples) and sediment PNECs.

Overall, the following 5 substances are finally proposed to be taken out of the 1st WL, based on the removal criteria and discussion: diclofenac, oxadiazon, 2,6-di-tert-butyl-4-methylphenol, tri-allate and 2-ethylhexyl-4-methoxycinnamate.

[12] Please note that 2 other substances would fulfil the criteria if the 2015 PNEC were taken into account (see details in Annex 6.1): azithromycin and thiamethoxam. The decrease in the updated PNEC for these substances explains the difference in the assessment (more than 3-fold decrease in the PNECs for each of these substances).

[13] Please note that the combined dataset is not relevant to assess the current risk posed by methiocarb. Methiocarb was banned as a molluscide in 2014, and consequently only data gathered after that date (e.g. from the WL dataset) would reflect the current level of risk. On the contrary, the combined dataset include samples dating back to 2006 which could overestimate the current level of risk for methiocarb. Consequently it shouldn't be taken into account when assessing whether there is sufficient high quality monitoring data to assess the risk for this substance.

[14] A partial ban on imidacloprid, clothianidin, and thiamethoxam was voted in 2013 with 2 conditions: The industrials needed to submit confirmatory data for remaining authorised uses and the commission should review the available evidence for all uses approved before the 2013 ban for these substances. A vote in the Standing Committee should take place in the coming months, on the basis of the EFSA's assessment of the data sent by the industrials. In parallel the EFSA is assessing the information gathered in a call launched to gather all available evidence, on all uses approved before the 2013 ban, and the report should be available in November.

[15] Recital 9 of Commission Implementing Decision 2015/495: "*For comparability, all substances should be monitored in whole water samples. However, it would be appropriate to monitor 2-ethylhexyl 4-methoxycinnamate also in suspended particulate matter or sediment, because of its tendency to partition into this matrix*."

Finally it was investigated if the lower updated PNEC values (given in Table 2) are achievable with current analytical methods. The analytical methods for the substances of the 1st WL were already reported in Loos (2015) and they were validated by Tavazzi et al. (2016). Table 6 shows that these lower PNECs should be achievable with good analytical instruments.

Table 6: Analytical achievement of updated PNECs.

Substance	**PNEC WL 2015 (µg/l)**	**Updated PNEC (µg/l)**	**Updated PNEC achievable with analytical methods proposed in Commission Implementing Decision 2015/495**
Clarithromycin	0.13	0.12	Yes; LOQ of Tavazzi et al. (2016) is 0.0046 µg/l; Several publications are given in Loos (2015).
Azithromycin	0.09	0.019	Yes; LOQ of Tavazzi et al. (2016) is 0.0026 µg/l; Several publications are given in Loos (2015).
Methiocarb	0.01	0.002	Yes; LOQ of SPE-LC-MS-MS method reported by Masiá et al. (2013) is 0.001 µg/l; LOQ of Tavazzi et al. (2016) is 0.00002 µg/l.
Imidacloprid	0.009	0.0083	Yes; LOQ of Tavazzi et al. (2016) is 0.001 µg/l; LOQ of SPE-LC-MS-MS method reported by Hladik et al. (2012; 2014) is 0.0049 µg/l.
Thiacloprid	0.05	0.01	Yes; LOQ of Tavazzi et al. (2016) is 0.00005 µg/l; LOQ of SPE-LC-MS-MS method reported by Hladik et al. (2012; 2014) is 0.0038 µg/l.
Thiamethoxam	0.14	0.042	Yes; LOQ of Tavazzi et al. (2016) is 0.001 µg/l; LOQ of SPE-LC-MS-MS method reported by Hladik et al. (2012; 2014) is 0.0039 µg/l.

Conclusions:

Table 7 lists the substances fulfilling all removal criteria, considering the WL dataset and updated PNECs. These are the following: diclofenac, clarithromycin, erythromycin, oxadiazon, tri-allate, 2,6-di-tert-butyl-4-methylphenol, acetamiprid, clothianidin, thiacloprid, and 2-ethylhexyl-4-methoxycinnamate.

The implementation of the removal criteria to the combined dataset together with updated PNECs confirms the above conclusions, except for thiacloprid.

However, to come to the final list of substances to be removed from the WL, the additional reasoning and information should be taken into account for neonicotinoids, macrolide antibiotics, and sunscreen ingredient (2-ethylhexyl-4-methoxycinnamate).

Overall, following the removal criteria and the additional discussion, 5 WL substances are proposed to be taken out of the list: diclofenac, oxadiazon, 2,6-di-tert-butyl-4-methylphenol, tri-allate, and 2-ethylhexyl-4-methoxycinnamate.

Table 7: Decision table on potential candidates to be removed from WL considering the WL dataset and updated PNEC values.

Notes:

1. The difference of the STE scores is calculated as a percentage by the formula $|STE_{Sc3} - STE_{Sc2}|/STE_{Sc3} * 100$
2. When $STE_{Sc3}=0$ and STE_{Sc2} is very low (<0.2) or =0 the difference of these scores is assumed to be zero

Substance	Updated PNEC (µg/L)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference <15%)	Potential candidate for deselection
Diclofenac	5.00E-02	Analgesic	9.90E-01	9.90E-01	25	6698	5.26	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Erythromycin	2.00E-01	Antibiotic	0.00E+00	0.00E+00	24	2520	0.14	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Clarithromycin	1.20E-01	Antibiotic	5.05E-01	5.05E-01	24	2792	1.45	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Azithromycin	1.90E-02	Antibiotic	8.79E-01	1.40E+00	19	915	4.49	50.5	no	59.65	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	0.00E+00	1.67E-01	23	1032	0.08	99.7	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
17-beta-Estradiol	4.00E-04	Estrogen	6.82E-01	1.17E+00	18	462	1.40	72.8	no	70.90	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Estrone	3.60E-03	Estrogen	5.42E-01	7.96E-01	20	552	0.97	91.6	yes	46.98	no	No (dissimilar STE scores)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	8.99E-01	1.91E+00	14	323	7.35	50.6	no	112.61	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Oxadiazon	8.80E-02	Herbicide	1.00E-01	1.01E-01	23	1847	0.45	99.9	yes	0.72	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Tri-allate	4.10E-01	Herbicide	0.00E+00	3.70E-04	23	2166	0.08	99.9	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Methiocarb	2.00E-03	Insecticide / Herbicide	1.20E-00	1.79E-00	7	127	0.83	6.6	no	48.77	no	No (no LOQ-PNEC criterion; dissimilar STE scores)

Substance	Updated PNEC (µg/L)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference <15%)	Potential candidate for deselection
Thiacloprid	1.00E-02	Neonicotinoid Insecticide	2.40E-01	2.51E-01	23	2235	1.00	99.6	yes	4.36	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Acetamiprid	5.00E-01	Neonicotinoid Insecticide	0.00E+00	0.00E+00	24	2221	0.02	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Imidacloprid	8.30E-03	Neonicotinoid Insecticide	7.53E-01	1.03E+00	22	1845	4.10	72.5	no	37.05	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Thiamethoxam	4.20E-02	Neonicotinoid Insecticide	7.64E-02	3.00E-01	23	3979	0.24	98.9	yes	292.39	no	No (dissimilar STE scores)
Clothianidin	1.30E-01	Neonicotinoid Insecticide	2.86E-01	2.86E-01	24	2254	0.25	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	0.00E+00	6.22E-04	23	543	0.50	99.3	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)

7.2 Selection of new substances for the 2nd WL

7.2.1 Criteria for including new substances in the 2nd WL

According to the EQSD, the Commission shall update the WL every 24 months. As a reminder, "the substances to be included in the watch list shall be selected from amongst those for which the information available indicates that they may pose a significant risk at Union level to, or via, the aquatic environment and for which monitoring data are insufficient" (EQSD article 8b). A reliable PNEC and an appropriate analytical method (LOQ below or equal to the PNEC) should be available for new substances included in the WL.

The criteria proposed here for the identification of new WL substances build on the technical work carried out for the review of the priority substances list led by the JRC with the support of the SG-R. During the review, substances with enough monitoring data to assess the risk they posed went through the so-called "monitoring-based approach", while others went through the modelling-based approach. Factsheets were drafted for substances ranking high through either of these approaches. On the basis of these factsheets, 10 substances were short-listed for further consideration (and in particular for EQS derivation).

For more details on the methodologies, please see the summary available at the following link: https://circabc.europa.eu/w/browse/0f6b893e-b0ab-46cb-a631-c3e1e55c7514

Respecting the requirements of the EQSD Directive, the JRC is proposing the following criteria for identifying potential candidates for inclusion in the 2nd WL:

Criteria based on the 2014 prioritisation:

1. Substances for which factsheets were prepared during the ongoing prioritisation process but not shortlisted because there were few or low-quality monitoring data.

2. Substances short-listed but with uncertainties for the monitoring data.

3. Substances considered in the modelling based exercise (Lettieri et al, 2016) for which:

    a. The monitoring data met the representativity criteria (number of MS, sites and samples) in Sc2 but not in Sc3, and

    b. In Sc2 the STE score was high and the modelled RQ was high.

4. Substances which went directly to the modelling stream (measured below 4 MS in Sc2 during the ongoing prioritisation) with modelled RQ above 5 but not further selected because of lack of monitoring data.

Additional criteria:

5. Substances identified as potentially relevant in the report "Development of the first Watch List" (Carvalho, et al., 2015), but not included in the 1st WL because of limitations in the information available at the time (e.g. on analytical methods).

6. Substances of emerging concern identified based on research projects and articles to identify substances of emerging concern, in line with the EQSD article 8b.

Please note that banned substances fulfilling the criteria above will not be taken into consideration as potential candidate for the WL following the final recommendation cited in the document on the development of the 1st Watch List.[16]

Please note also that a further scrutiny of the substances identified with these criteria has been carried out. This further scrutiny included consideration of other information such as

[16] Development of the 1st Watch List under the Environmental Quality Standards Directive - Document for 2nd Meeting of WFD CIS Working Group Chemicals, 17-18 March 2014 (DG ENV).

the number of MS in which the substance is authorised, a comparison of the RQ and/or STE scores between the different substances, to establish a priority for the inclusion in the WL, the consideration of the relevant matrix and stability of the substance (see details in Annex 9), in addition to the consideration of the availability of a reliable PNEC and an appropriate analytical method. These elements are presented below.

7.2.2 Identification of new substances for inclusion in the 2nd WL

Based on criterion 1, chromium (VI) and teflubenzuron are potential candidates. Teflubenzuron was not shortlisted during the previous prioritisation because the monitoring data were considered to be insufficient. For chromium (VI) the available monitoring data (Sc3) in the 2014 prioritisation exercise were from "whole water" (not filtered); monitoring data quality and quantity were very low. Furthermore the risk quotient (RQ) based on predicted environmental concentration (PEC, Carvalho et al., 2015) was 102.9, although this value probably overestimated the risk because it didn't take into account the restrictions recently imposed on the uses of chromium under REACH (see Table 10). Consequently this substance was initially proposed for the WL, however in January 2018 the JRC received more recent monitoring data for total chromium in dissolved fraction from several Member States, as well as additional monitoring data for chromium (VI) in dissolved fraction from one Member State. All these data were for inland waters (rivers and lakes). Furthermore, the JRC reviewed the ecotoxicological data available not only for chromium (VI) but also for chromium (III). This led to an update for the PNEC in freshwaters of 2.06 μg/l and 1.8 μg/l for chromium (VI) and chromium (III) respectively (see more details in the chromium factsheet, annex 9). Based on the updated PNEC (2.06 μg/l) the RQ for chromium (VI) has been approximated considering the total chromium concentrations in dissolved phase (based on all monitoring data available, from 2010 onwards, in inland waters). This RQ is however below 1 (RQ(P95)=0.49), which doesn't tend to support the inclusion of chromium (VI) in the WL. The same calculation was performed with the PNEC for chromium (III) (1.8 μg/l), leading to the same conclusion (RQ(P95)=0.56). Finally, the JRC derived a PNEC for coastal and transitional waters for chromium (VI). Based on this PNEC (0.6 μg/l) and on the monitoring data used in the prioritisation for total chromium in dissolved fraction (coastal and transitional waters), the RQ(P(95) is 1.17, which warrants further investigation (see chromium factsheet, annex 9). In addition, before any definitive conclusion can be made, the PNECs derived by the JRC will need to be confirmed, via consultation with the WG Chemicals.

Based on criterion 2, in the summary document of the prioritisation exercise[17], the table summarising conclusions from the 6th SG-R meeting, shows the certainty/uncertainty for each substance shortlisted as potential PS candidate. Silver, omethoate, selenium and the pyrethroids were identified as having a low/medium amount of monitoring data in the prioritisation. Silver, omethoate and selenium are not proposed as WL substances. According to the latest information available at the moment, dated 2014[18], silver, omethoate and selenium (in water) are RBSPs in a significant number of MS (resp. 7, 6 and 10 MSs). This tends to support the idea of an EU-wide risk. In addition, more monitoring data should become available via routine monitoring in the future, in particular for silver and omethoate. What's more, the additional monitoring data recently gathered combined with the data previously used in the prioritisation now show more than 2000 samples in more than 100 sites and 4 MS for silver in the dissolved fraction, so it fulfils the minimum requirements for the number of MS, sites and samples used under the previous prioritisation. For selenium, the SG-R deemed that the most relevant matrix for monitoring and assessment is biota: a QS biota needs to be developed before additional information can be gathered in this matrix.

[17] https://circabc.europa.eu/w/browse/0f6b893e-b0ab-46cb-a631-c3e1e55c7514
[18] More recent information will be available once the 2nd RBMPs have been fully analysed.

The pyrethroids permethrin, deltamethrin, bifenthrin and esfenvalerate were all shortlisted and although three of them were selected from the modelling based exercise, the criteria for their selection were not only based on the modelled RQ but also on realistic scenario for PEC derivation, ratio between PEC RQ and MEC RQ (close to 1) and additional monitoring data (see Lettieri et al, 2016). Furthermore permethrin and deltamethrin were already identified in the previous exercise. During the 6th SG-R meeting, experts were split between inclusion in the priority substances list or in the Watch list, provided an adapted analytical method would be developed. Consequently the JRC suggests that when an adapted analytical method is made available for these substances, they can be considered in a further update of the list.

Under the criterion 3, the substances from the previous prioritisation with sufficient monitoring data in Sc2 but not in Sc3 (data in less than 4 MS) are considered. These substances went through the modelling-based exercise. Among these substances, those with a high modelled RQ AND a high STE score in Sc2 can be considered for inclusion in the 2nd WL (criterion 3). There were 16 substances in this case (for details see page 51 of the report, Lettieri et al., 2016). From the list the banned substances and the three shortlisted substances (deltamethrin, bifenthrin and esfenvalerate) were removed. Other substances fulfilling criterion 3 are shown in Table 8. They are teflubenzuron (already selected under criterion 1), and diflubenzuron.

Considering the criterion 4, the Table 9 shows substances which went directly to the modelling stream (measured below 4 MS in Sc2 during the ongoing prioritisation) and which modelled RQ is higher than 5. They are pyridaben, dimoxystrobin, etofenprox, fenpyroximate and thiram, chlorsulfuron, metconazole, metaflumizone, proquinazide, diflubenzuron, and venlafaxine.

Table 8: List of substances identified as potential candidates for the WL under criterion 3. These are substances:

- from the previous prioritisation with sufficient monitoring data in Sc2 but not in Sc3. (These substances went through the modelling-based exercise) AND

- with a high modelled RQ and a high STE score in Sc2 can be considered for inclusion in the 2nd WL, AND

- which are still approved

Please note the three shortlisted substances (deltamethrin, bifenthrin and esfenvalerate) fulfil these criteria but are not included in this table because they already fulfil criteria 2.

Please note also that because the RQ(MEC95) are based on data of insufficient quality and quantity, these cannot be considered as reliable.

SUBSTANCE	Type	PEC (µg/l)	PNEC (µg/l)	PEC RQ	Hazard	STE score	RQ(MEC P95)	Monitoring No. MS in sc3	Monitoring No. Sites	Monitoring No. Samples	No. Samples < LOQ	No. Quantified samples	Status
Teflubenzuron	PPP	4.62	0.0012	3847	PBT	2.28	41.7	1	1	9	0	9	Approved
Diflubenzuron	PPP, Biocide	13.62	0.004	3406	T	1.22	0.6	2	13	218	0	218	Approved

Table 9: List of substances with monitoring data in Sc2 from less than 2 MS, and which modelled RQ is higher than 5 (criteria 4).

Please note that this table has been extracted directly from the monitoring based report for the 2014 prioritisation. The PNEC for the substances of interest have been reviewed, which may lead to differences between the PNEC mentioned here and the PNEC mentioned in the following tables.

Please note also that because the RQ(MEC95) are based on data of insufficient quality and quantity, these cannot be considered as reliable.

Substance	Type	PEC (µg/l)	PNEC (µg/l)	RQ(PEC)	Hazard	STE score	RQ(MEC P95)	Monitoring No. MS in Sc2	Monitoring No. Sites	Monitoring No. Samples	No. Samples < LOQ	No. Quantified samples	Status
Pyridaben	PPP	10.40	0.00047	22132	PBT	2.41	53[19]	2	785	5395	5395	0	Approved
Dimoxystrobin	PPP	16.42	0.0032	5196	PT, suspected C, R	2.13	8	1	720	6078	5910	168	Approved
Etofenprox	Biocide (ECHA) Plant protection product	8.3	0.0054	1531	B, T suspected R	1.52	1.85	3	91	1116	1106	10	Approved
Fenpyroximate	PPP	4.4	0.010	440	PBT	0	1	1	35	1506	1505	1	Approved
Thiram	Industrial (ECHA) Biocide (ECHA) Plant protection product	61.0	0.200	305	T , ED	0	0.25	3	217	3546	3534	12	Approved
Chlorsulfuron	PPP	2.9	0.024	119	P, T , suspected C	0.84	1.04	3	1239	15973	15	49	Approved

[19] No samples were quantified. This RQ above one is an artefact resulting from the use of LOQ/2 for non-quantified samples.

Metconazole	PPP	5.9	0.0582	101	PT, vP, suspected R	0	0.43	3	702	5742	5739	3	Approved
Metaflumizone	PPP	0.3	0.01308	22.8	P, B, T	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	Approved
Proquinazide	PPP	1.3	0.18	7.28	vP, B and T	0	0.06[20]	1	31	1285	1285	0	Approved
Diflubenzuron	PPP, biocide	13.62	0.004	3406	P, B, T	2.09	6.25	4	415	4725	4607	2	Approved
Venlafaxine	Human medicine	0.20	0.038	5.21	P, T	1.36	4.95	1	93	1395	324	1071	Approved

[20] No samples were quantified. This RQ above one is an artefact resulting from the use of LOQ/2 for non-quantified samples.

Criterion 5 is to consider also substances included in the report "Development of the first Watch List" (Carvalho, et al., 2015); in this report the substance free cyanide (CN^-) was listed however it was not selected because a good analytical method was not available. A study carried by Fraunhofer Institute in collaboration with the Stakeholder Consortia (Cefic Cyanide Sector Group, CONCAWE, EUROFER and Euromines) succeeded to set up the analytical method. Furthermore CN^- has been also shortlisted in the first prioritsation exercise and an updated draft dossier is available in CIRCABC[21].

Criterion 6 is to consider also substances of emerging concerns, highlighted by research projects and scientific articles (in line with the requirements of EQSD article 8b). From this source, three antibiotics have been selected because of the potential risk they pose to the aquatic environment highlighted by scientific pulbications, and because of the emerging concern of antibiotic resistance: Amoxicillin and ciprofloxacin. The selection of these antibiotics is also in line with the European One Health Action Plan against antimicrobial resistance.[22]

Wang et al. (2017) found high ecological hazards of mixture of antibiotics mainly for algae. Tetracycline, oxytetracycline, sulfadiazine, and ciprofloxacin pose medium to high hazards to algae.

Quinlan et al. (2011) have reported that significant changes in the stream biotic community were observed within 7 days with in-stream tetracycline concentrations as low as 0.5 µg/L, including significant changes in antibiotic resistance, bacteria abundance and productivity, algae biomass, cyanobacteria, organic biomass, and nematodes.

The references to additional publications are detailed in the facstheets for these substances in Annex 9.

In conclusion, the Table 10 lists the substances identified on the basis of the 6 above criteria for further scrutiny. The table includes where relevant for each substance the dates by which the approval should be reviewed, and number of MS in which it is approved.

Furthermore in the table are reported the PNEC values, STE score for the substances selected from the monitoring based exercise and those from the Table 9. For the modelled substances, the PEC, the RQ, hazard properties and number of MS where it is authorised are reported. The column to the right includes additional comments.

Among these substances the JRC wouldn't recommend thiram, famoxadone, metconazole, fenpyroximate, dimoxystrobin and chlorsulfuron for inclusion in the 2nd WL because of the dates for expiration of their approval between 2018 and 2019, respectively. The JRC also doesn't recommend to include teflubenzuron in the WL because it is authorised only in 4 MS.

[21] Draft Dossier for free cyanide is available on CIRCABC: https://circabc.europa.eu/w/browse/31cc6882-0faf-4826-a61b-39b81a4c2c5c

[22] The Action Plan states: "maximise the use of data from existing monitoring, e.g. Watch List monitoring under the Water Framework Directive, to improve knowledge of the occurrence and spread of antimicrobials in the environment"

Table 10*:* List of substances fulfilling either of the 6 above criteria for identification as potential candidate for inclusion in the 2nd WL. In bold the STE score and modelled RQ (PEC/PNEC) for substances from the monitoring based exercise and modelling based exercise respectively. For free cyanide and the antibiotics amoxicillin and tetracycline the RQ is the ratio of Measured Environmental Concentration (MEC) and the PNEC since no PEC is available. Additional information have been included i.e. monitoring data.

Substance	**PNEC (µg/l)**	**STE score and RQ**	**Monitoring data (MSs, number of sites and samples)**	**Comment**
Chromium (VI)	2.06[1]	**RQ (102.94)** **RQ(MEC)=2.43** **STE=1.1** See p. 61 for more information on the approximation of RQ(MEC) using monitoring data for total chromium.	In Sc3 for inland whole water (monitoring-based prioritisation 2014-2016), 753 samples were available from 4 countries, 51 % of them quantified.	Predicted Environmental Concentration (PEC) has been derived before the restricted use therefore it overestimates the risk .The available monitoring data in the prioritisation exercise were from "whole water"; Monitoring data quality and quantity is very low.
Metaflumizone	0.0654[1]	PEC 0.3 **(RQ 4.6)** vP, vB and T (hazard properties)	No monitoring data Authorised as PPP in 13 MS 1 is in progress	Approved until 31/12/2024
Amoxicillin	0.078[1]	**RQ (MEC) 1.28**	In Sc2 for inland whole water (monitoring-based prioritisation 2014-2016), 86 samples from 1 country	Data quality is not good
Ciprofloxacin	0.089[4]	PEC 7 (RQ 84.2) T (hazard properties)	In Sc2 data from 3 MS (54 sites) with 842 samples are available. 9% are quantified.	Data quality is not good
Etofenprox	0.00108[1]	PEC 8.3 (**RQ 1531**) B, T suspected R (hazard properties)	Monitoring data only from 3 MS with 91 site and 1316 samples. Only1 quantified samples Etofenprox is authorised in 18 MS; in 10 MS as a PPP (BG, CZ, EL, ES, HU, MT, PL, RO, SK, UK), in 4 MS as a PPP and as a biocide (AT, DE, FR, IT) and in 4 MS as a biocide (DK, LU, SE, SI)	Monitoring data as supportive information not sufficient to bring forward in the prioritisation Expiration of approval (as a PPP): 31/12/2019 Biocidal active substance: 8-Wood Preservatives,

Substance	PNEC (µg/l)	STE score and RQ	Monitoring data (MSs, number of sites and samples)	Comment
				expiry date 01/02/2020 18- Insecticide, acaricides and products to control other arthropods, expiry date 01/07/2025
Dimoxystrobin	0.03[6]	PEC 16.42 (**RQ 519.6**) PT (hazard properties)	Monitoring data only from 1 MS with 720 site and 6078 samples. 2.8 % quantified samples Authorised in 16 MS	Monitoring data as supportive information not sufficient to bring forward in the prioritisation Expiration of approval: expiration date has been extended by one year for until 31/01/2019
Proquinazid	0.18[4]	PEC 1.3 **(RQ 7.28)** vP, B and T (hazard properties)	Data from only 1 MS (31 sites) with 1285 samples are available. No quantified samples. Authorised as PPP in 24 MS and 1 pending	Approved until 31/07/2020
Venlafaxine	0.038	PEC 0.20 **(RQ 5.21)** P, T(hazard properties)	Data from 1 MS (93 sites) with 1395 samples are available in Sc2. 76.8% quantified samples	EOTOX data from EPA but the study not available.
Free Cyanide	0.5[9]	RQ 10-40 (MEC (5-20)[10] T (hazard properties)	No monitoring data from the prioritisation exercise	
Pyridaben	0.0047[1]	PEC 10.40 (**RQ 2212**) PBT[2] (hazard properties)	Monitoring data only from 2 MS with 785 site and 5395 samples. No quantified samples Authorised in 11 MS	Monitoring data as supportive information not sufficient to bring forward in the prioritisation Expiration of approval: 30/04/2021
Fenpyroximate	0.010[1]	PEC 4.4 (**RQ 440**) PBT[3] (hazard properties)	Monitoring data only from 3 MS with 91site and 1316 samples. Only1 quantified samples Authorised in in 18 MS	Monitoring data as supportive information not sufficient to bring forward in the prioritisation

Substance	PNEC (µg/l)	STE score and RQ	Monitoring data (MSs, number of sites and samples)	Comment
				Expiration of approval: 30/04/2019
Diflubenzuron	0.0008[1]	PEC 13.62 (**RQ 3406**) **STE=1.2 (Sc2)** T (hazard properties)	Monitoring data from 4 MSs with 415 sites and 4725 samples in Sc2 while 2 MSs with 13 sites and 218 samples in Sc3 Authorised in 20 MS (in 16 MS as a PPP, in 3 MS as a biocide, in 1 MS as a PPP and as a biocide)	Monitoring data are very few not sufficient as supportive information to bring forward in the prioritisation Expiration of approval (as a PPP): 31/12/2018 Biocidal active substance: 18- Insecticide, acaricides and products to control other arthropods, expiry date 01/02/2025
Thiram	0.2[4]	PEC 61 (**RQ 305**) T (hazard properties[5])	Monitoring data only from 3 MS with 217 site and 3546 samples. Authorised in 24 MS	The available data although not sufficient for STE run, is good since the LOQ is below the PNEC value. The MEC RQ is 0.25 suggesting that the modelled RQ is not supported by the monitoring data so far available from 3 MS. Expiration of approval: 30/04/2018 Biocidal active substance: Approval status under review by 1 MS (BE)
Teflubenzuron	0.0012	PEC 4.62 (**RQ 3847**) STE =2.8 (Sc2) PBT[8] (hazard properties)	The number of monitoring samples, from 4 MSs in Sc2 is 7000 with almost all of them below LOQ (range 0.005-0.05) and none below LOD. Only 9 quantified samples from 1 MS are available (Sc3). Authorised in 4 MS	Factsheet for this substance was prepared but it was not put forward for EQS derivation, after SG-R comments, because the monitoring data were considered to be not sufficient, and

Substance	PNEC (µg/l)	STE score and RQ	Monitoring data (MSs, number of sites and samples)	Comment
				therefore as EU-wide concern for freshwater is not proven Expiration of approval: 30/11/2019
Chlorsulfuron	0.024[4]	PEC 2.9 (RQ 119) P T suspect C (hazard properties)	Data from 3 MS with 1239 site and 15973, only 0.31% quantified) Authorised in 9 MS	Until 31/12/2019.
Metconazole	0.0582	PEC 5.9 (RQ 101) vP T suspect R (hazard properties)	Data from 3 MS (702 site with 5742 samples and 0.05 % quantified samples) Authorised in 24 MS	Approved until 30/04/2018 – Although the expire date is in April 2018, it is vP and should be monitored
Famoxadone	0.14[1]	PEC 1.8 (RQ 12.6) B, T (hazard properties)	Data from 3 MS Authorised as PPP in 18 MS	30/06/2018 Although the expire date is in June 2018, still good candidate since it is B as hazard property

[1] JRC Derivation

[2] EFSA Dossier 2010

[3] P/B: EFSA Dossier 2013; T: CL Inventory

[4] Oekotoxzentrum, Eawag/EPFL (CH)

[5] In 2015 the Sweden stated that "*In the light of general systemic toxicity, the available data set does not allow concluding that thiram alters function of the endocrine system and consequently causes adverse health effects*". Conclusion document online: https://echa.europa.eu/it/information-on-chemicals/evaluation/community-rolling-action-plan/corap-table/-/dislist/details/0b0236e18070b8fd

[6] ETOX: Information System Ecotoxicology and Environmental Quality Targets (UBA)

[7] EU Report 2012

[8] EFSA Dossier 2008

[9] Draft Dossier for free cyanide is available on CIRCABC: https://circabc.europa.eu/w/browse/31cc6882-0faf-4826-a61b-39b81a4c2c5c

[10] MEC source from NORMAN Database http://www.norman-network.net/?q=node/24 and WATERBASE Database http://www.eea.europa.eu/data-and-maps/data/waterbase-rivers-6

Table 11 shows the final list of recommended substances that are potential candidates for inclusion in the 2nd or 3rd WL. The first three substances in the table (metaflumizone, amoxicillin and ciprofloxacin) are recommended for inclusion in the 2nd WL. The following substances are recommended for consideration for the 3rd WL. The PNECs, available analytical methods, and if the lowest LOQ is below the PNEC are shown.

Separate factsheets have been prepared for each substance (Annex 9). The factsheets give information on substance identity, physico-chemical properties, environmental fate, environmental exposure (PECs/MECs), analytical methods, P, B, T, C, M, R, ED properties, ecotoxicology data, PNEC derivation, risk quotients and STE scores (if available).

The preferred monitoring matrix for the hydrophobic substances (pyrethroid insecticides; pyridaben) with high log K_{OW} values is sediment or biota.

Table 11: Summary of analytical methods and reliability of the PNECs for the potential WL candidate substances.

Substance	CAS	PNEC (µg/l)	Is the PNEC reliable	Available analytical method for analysis in water	LOQ < PNEC (in water)
Metaflumizone	139968-49-3	0.0654	Yes	LC-MS-MS	Yes (LOQ = 0.025)
Amoxicillin	26787-78-0	0.078	Yes	LC-MS-MS	Yes (LOQ = 0.004)
Ciprofloxacin	85721-33-1	0.089	Yes	LC-MS-MS	Yes (LOQ = 0.002)
Chromium (VI)	18540-29-9	2.06 (inland surface waters); 0.6 (transitional and coastal waters)	Yes	EPA method 218.7; Ion chromatography followed by post-column derivatization of the Cr(VI) with diphenylcarbazide and detection of the colored complex at 530 nm; LC-ICP-MS	Yes
Etofenprox	80844-07-1	0.00108 [2]	Yes	GC-ECD-MS or GC-MS	?[23]
Dimoxystrobin	149961-52-4	0.0316	Yes	LC-MS-MS	Yes (LOQ = 0.01)
Proquinazide	189278-12-4	0.18	No	GC-MS	Yes (LOQ = 0.1)
Venlafaxine	93413-69-5	0.038	No	LC-MS-MS	Yes (LOQ = 0.0003)
Free Cyanide	57-12-5	0.5	Yes	CFA-photometric detection	Yes[24]
Permethrin	52645-53-1	0.00047	Yes	HRGC-HRMS	Yes (LOQ = 0.000044)
Esfenvalerate	66230-04-4	0.0001	Yes	GC-NCI-MS	Yes (LOQ = PNEC)
Pyridaben	96489-71-3	0.0047 [2]	Yes	LC-MS-MS	No (LOQ = 0.005)
Fenpyroximate	134098-61-6	0.01 [2]	Yes	LC-MS-MS	No (LOQ = 0.1)
Diflubenzuron	35367-38-5	0.0008 [1]	Yes	LC-MS-MS	No (LOQ = 0.04)
Deltamethrin	52918-63-5	0.00007	Yes	GC-ECD/MS or GC-NCI-MS	?[25]
Bifenthrin	82657-04-3	0.00002	Yes	GC-ECD/MS or GC-NCI-MS	?[25]

[1] EU Report 2012

[2] JRC Derivation

[23] One publication from China was found giving a multi-compound analytical method for 82 pesticides; the general LOD of 0.00006–0.00098 µg/l given is questionable (Zheng et al., 2016).

[24] An LOQ of ca. 0.14-0.30 µg/l was reached. Natural background concentrations between 0.127-0.240 µg/l were determined in Germany (Fraunhofer Institute, 2017).

Conclusion:

Taking into account the availability of an appropriate analytical method (LOQ at least as low as the PNEC) and of a reliable PNEC, JRC would recommend for the 2nd WL metaflumizone, amoxicillin and ciprofloxacin.

Other substances such as pyrethroids (etofenprox, permethrin, esfenvalerate, deltamethrin and bifenthrin) and pyridaben would be interesting to consider in a following update of the list (e.g. 3rd WL) to be measured in the most appropriate matrix. Furthermore venlafaxine and proquinazid should be also considered if reliable information for the PNEC is found. Free cyanide should also be considered when the analytical method recently developed is made available. No appropriate analytical method has been found for diflubenzuron and fenpyroximate. In addition, the approval of dimoxystrobin as a PPP should be reviewed by January 2019. If the approval for this substance is renewed, then it can be considered for inclusion in the 3rd WL. Furthermore, upon confirmation of the PNEC derived for chromium (VI) and (III) by consulting with the WG Chemicals, the JRC will also further investigate a potential risk posed by chromium (VI) in coastal and transitional waters, in particular by investigating whether monitoring data more recent than those used in the prioritisation are available, in view of a possible inclusion of chromium (VI) in the 3rd WL. Finally, thiram, metconazole and famoxadone could be considered for inclusion in the 3rd WL if their approval is renewed and if a reliable PNEC and an appropriate analytical method are available.

8 Conclusions

Based on the performed analyses, we could conclude that the first WFD watch list program has fulfilled its objective of gathering Union-wide high-quality surface water monitoring data for several of the selected substances.

Nearly all EU Member States have provided monitoring data of mostly good quality. Analytical method performance improvements would however be necessary in some MS for 17-alpha-ethinylestradiol (EE2), 17-beta-estradiol (E2), imidacloprid, azithromycin, and methiocarb (for the updated PNECs).

Around half of the MS did not give the relevant information on the representativity of the monitoring stations and monitoring strategy including the nearby pressures of the sampling stations. This information would be necessary for a better interpretation of the WL data.

Sampling site selection and correct timing of sample collection is essential for monitoring of plant protection products (PPPs) because exposure of surface waters to pesticides is heavily dependent on local conditions (e.g. pesticide application and land use) and therefore can be spatially and temporally variable. In addition, antibiotics show an increased use during winter and the sunscreen ingredient in the summer. Only one MS provided in their sampling strategy detailed information on the timing of sample collection.

JRC has identified 10 substances, based on the criteria defined, as potential candidates to be removed from the first WL when considering the WL dataset together with the updated PNECs: diclofenac, clarithromycin, erythromycin, oxadiazon, tri-allate, 2,6-di-tert-butyl-4-methylphenol, acetamiprid, clothianidin, thiacloprid, and 2-ethylhexyl-4-methoxycinnamate.

The potential candidates for removal from the WL were confirmed applying the removal criteria to the combined dataset together with updated PNECs except for thiacloprid.

Despite the above, there are reasons for retaining some of the substances in the WL, as explained in the main part of the document (section 7.1).

Consequently only diclofenac, oxadiazon, 2,6-di-tert-butyl-4-methylphenol, tri-allate and 2-ethylhexyl-4-methoxycinnamate are proposed to be removed from the first WL.

Based on the criteria identified in section 7.2 above, JRC proposes to select as a new WL substances for inclusion in the 2nd WL the following substances from the prioritisation monitoring and modelling exercise 2016 with low monitoring data quality and quantity, which are: metaflumizone, amoxicillin and ciprofloxacin. Please note that in selecting these substances, additional information, such as the date of expiration of their approval and the number of MS where they are approved, the available analytical method with LOQ < PNEC and the matrix have been taken into account.

In addition, when an adequate analytical method is available and possibly by measuring in the most appropriate matrix (i.e. sediment or biota) the pyrethroid insecticides (etofenprox, permethrin, deltamethrin, bifenthrin and esfenvalerate), and pyridaben could be proposed as group of substances to be included in the WL for its next update. Furthermore venlafaxine and proquinazid should be also considered when reliable information for PNEC is made available. Free cyanide should also be considered when the analytical method recently developed is made available. Finally, the approval of dimoxystrobin as a PPP should be reviewed by January 2019. If the approval for this substance is renewed, then it can be considered for inclusion in the 3rd WL. Chromium (VI) is not proposed for inclusion in the 2nd WL. The JRC's assessment of the new monitoring data received in January 2018 together with the data from the 2014 prioritisation doesn't support the idea that chromium (VI) would be posing a risk in freshwaters. However, chromium (VI) could be considered for inclusion in the 3rd watch list in transitional and coastal waters, after confirmation of the PNEC via consultation with the WG Chemicals and after collection and analysis of any additional existing monitoring

data for these categories of water. Finally, thiram, metconazole and famoxadone could be considered for inclusion in the 3rd WL if their approval is renewed and if a reliable PNEC and an appropriate analytical method are available.

References

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List of abbreviations and definitions

CAS	Chemical Abstract Service
EEA	European Environment Agency
EE2	17-alpha-Ethinylestradiol
E1	Estrone
E2	17-beta-Estradiol
EFTA	European Free Trade Association
EQS	Environmental quality standard
GC-MS	Gas chromatography mass spectrometry
LC-MS-MS	Liquid chromatography (tandem) triple quadrupole mass spectrometry
LLE	Liquid liquid extraction
LOQ	Limit of quantification
MS	Member State
PEC	Predicted environmental concentration
PNEC	Predicted no-effect concentration
MEC	Measured environmental concentration
PPP	Plant protection product
RQ	Risk Quotient
SG-R	Sub-group on revision (of the priority substance list)
SoE	State of the Environment
SPE	Solid-phase extraction
SPM	Suspended particle matter
STE	Spatial, Temporal and Extent of PNEC exceedance
WFD	Water Framework Directive
WISE	Water Information System for Europe

The European ISO country codes can be found online:
http://ec.europa.eu/eurostat/statistics-explained/index.php/Glossary:Country_codes

List of figures

List of tables

Supplementary Information

The annexes below present a detailed information (tabular and/or graphical) for the different datasets about the data statistics, range of LOQs, quality of data, STE scores, STE factors, the removal of substances from WL, the inclusion of new substances to the WL and additional information individually for WL substances (nearby pressures, seasonality and distribution per country).

Annex 1: STE assessment tool

For the monitoring-based prioritisation exercise, the Joint Research Centre (JRC) of the European Commission (EC) developed a chemical risk assessment tool, called "Spatial, Temporal and Extent of exceedance" (STE), which accounts the concentration exceedances over the Predicted No Effect Concentration (PNEC) considered as an eco-toxicological threshold of concern (Carvalho et al., 2016).

The STE method follows the concept of von der Ohe et al. (2011), where substances were assessed as potential river basin specific pollutants based on two indicators - the spatial frequency of PNEC exceedances, considering the maximal concentrations at different monitoring sites, and the extent of the PNEC exceedance, considering the absolute risk ratio to evaluate the intensity of local impacts (using 95th percentile of max concentration at each monitoring site).

The STE method introduced modifications on the originally proposed calculations for the Spatial and Extent factors - the max concentration was substituted by 95th percentile of concentrations when accounting the exceedances at monitoring sites. Moreover, in the Spatial factor a correction of the frequency of exceedances at sites was established by the percentage of the countries with exceedances. In addition a new temporal factor has been included to further explore the inherent variability of the monitoring data and to improve the ranking of substances. Moreover, the robustness and sensitivity of the STE method were tested, in particular with respect to the quantity and quality of the monitoring data, and the statistical independence of the individual STE factors and the impact of uncertainty of the PNEC values were verified (Carvalho et al., 2016).

The STE method calculates for each substance an overall risk assessment score by summing the Spatial, Temporal and Extent of PNEC exceedance factors. 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 an extremely high concern. In the prioritisation exercise (that started in 2014) 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 the table below.

STE score	Risk classification
≥ 2.4 and ≤3	Very high
≥ 1.8 and < 2.4	High
≥ 1.2 and < 1.8	Intermediate
≥ 0.6 and < 1.2	Low
≥ 0 and < 0.6	Very low

Then, the substances showing high and very high risks (i.e. STE ≥ 1.8) were short-listed and eventually proposed as new candidates for priority substances.

Advantages of the STE method:

a) Simplicity

The method is built on a simple and distinct scheme that calculates Spatial, Temporal and Extent factors of exceedances per substance using measurements in different environmental compartments (water, biota, sediment, etc.) and identifies when a potential risk exists comparing to EQS/PNEC values.

b) Robustness

The STE factors are sound and robust indexes for quantification of spatial, temporal and extent of eco-toxicological exceedances.

The STE factors are confirmed being independent from a statistical point of view by the Chi-squared test for statistical independence and low correlations among them.

The statistical independence of the STE factors allows summing of the spatial, temporal and extent factors in a single and representative final score for each substance.

c) Novelty and Innovation

An additional term for the exceedances per country was added to the spatial factor. It plays an extra controlling role on the spatial propagation of the impact of toxic chemicals at continental scale.

A new temporal factor was introduced in the chemical risk assessment since some substances could present sudden peak concentrations or are affected by clear seasonality.

A better quantification of the extent of exceedance factor was developed which guarantees that the extent factor increases more gradually and smoothly.

Shortcomings of the STE method:

a) Data quality

Since the outcome of STE method is susceptible to the quality and quantity of monitoring data they should be subject to a strict evaluation according to a set of general requirements and criteria for quantification limits, representativity and treatment of outliers.

b) Sensitivity

The method showed a low sensitivity to the number of samples and sites where substances are measured (in case they are sufficient statistically). However, before applying the STE method a detailed statistical analysis of datasets is always needed in order to avoid inconsistent and unrealistic outcome. In particular, it is important to check if a sufficient number of measurement stations and records per substance are available that for example could be measured occasionally or just once at some sites. Thus, it is important to set requirements on data for the minimum number of countries and sites with measurements, for the statistically sufficient number of samples, and for a minimal number of samples per site.

Conversely, the STE method is very sensitive to the choice and the uncertainty in the EQS/PNEC values which apparently are a very important parameters in the assessment of chemicals.

In conclusion, STE method is a robust and innovative approach to rank substances in the chemicals risk assessment. When reliable data are available (measurements and EQS/PNEC values) STE could be applied for a variety of environmental compartments or receptors including surface and marine waters, sediment, biota, groundwater, and drinking water.

Annex 2: Sediment and SPM monitoring data

Monitoring data on sediment were submitted by five countries. Substances detected in sediment were 2-ethylhexyl-4-methoxycinnamate (countries #07, #09 and #29), clarithromycin (country #06), and diclofenac (only once detected in country #06).

The maximum concentration detected for 2-ethylhexyl-4-methoxycinnamate in sediment was 35 µg/kg, and therefore did not exceed the PNEC of 200 µg/kg. The total number of samples was 31.

Annex 2.1 Summary on sediment monitoring data.

Country	# of samples	Substances	Results
#06	290 (years 2014-2016)	Clarithromycin Diclofenac Erythromycin Triallate	Clarithromycin: often detected above the LOQ (2 µg/kg); mean: 6.5 µg/kg; max.: 65 µg/kg. Diclofenac: Only detected once above the LOQ of 10 µg/kg. Erythromycin: Not detected above the LOQ of 10 µg/kg. Triallate: Not detected above the LOQ of 10 µg/kg.
#07	11	2-Ethylhexyl-4-methoxycinnamate	All monitoring data on 2-ethylhexyl-4-methoxycinnamate in sediment were below the LOQ, which was between 2 and 10 µg/kg. No information on nearby pressure "bathing site" was given. (number of samples: 11)
#09	68	17-alpha-Ethinylestradiol 17-beta-Estradiol 2,6-Ditert-butyl-4-methylphenol 2-Ethylhexyl-4-methoxycinnamate Azithromycin Clarithromycin Diclofenac Erythromycin Estrone Triallate	All measurements except one (for 2-ethylhexyl 4-methoxycinnamate) were below the LOD. 2-Ethylhexyl-4-methoxycinnamate was detected at one monitoring site at a concentration of 8.5 µg/kg dry weight. No information on nearby pressure "bathing site" was given. (number of samples: 4)
#26	18	2,6-Ditert-butyl-4-methylphenol 2-Ethylhexyl-4-methoxycinnamate Triallate	Three substances were measured at 6 locations. All data were below the LOQ. 2,6-Ditert-butyl-4-methylphenol: LOQ 0.5 µg/kg; 2-Ethylhexyl-4-methoxycinnamate: LOQ 0.2 µg/kg;

Country	# of samples	Substances	Results
			Triallate: LOQ 0.5 µg/kg.
#29	16	2-Ethylhexyl-4-methoxycinnamate	2-Ethylhexyl-4-methoxycinnamate was detected 6 times (out of 16 samples) above the LOQ of 7 µg/kg. The maximum concentration was 35 µg/kg. No information on nearby pressure "bathing site" was given. A screening study was undertaken in 2014; most samples were taken close to recreational bathing sites. A more detailed study in a small lake with popular bathing sites where surface water and sediment were sampled before, during and after the bathing season. In addition surface water and sediment samples were taken upstream and downstream a STP effluent point. In an earlier screening study, several sites were sampled before and during the bathing season. Results from that study have been reported to JRC previously.

In addition, SPM (suspended particle matter) monitoring data were submitted by country #6 for clarithromycin, diclofenac, erythromycin, and triallate (years 2014-2016). Only clarithromycin was detected above the LOQ (median concentration: 39 µg/kg) (see table below).

Annex 2.2 Summary on SPM monitoring data of country #6 (concentrations in µg/kg).

Substance	Number of samples	LOQ	Min	Median	Mean	Max	Comment
Clarithromycin	11	2	12.0	39.0	45.4	93.0	All samples > LOQ
Diclofenac	11	10	n.a.	n.a.	n.a.	n.a.	All samples < LOQ
Erythromycin	11	10	n.a.	n.a.	n.a.	n.a.	All samples < LOQ
Triallate	549	10	n.a.	n.a.	n.a.	n.a.	All samples < LOQ

Annex 3: Detailed statistics for WL substances by WL dataset

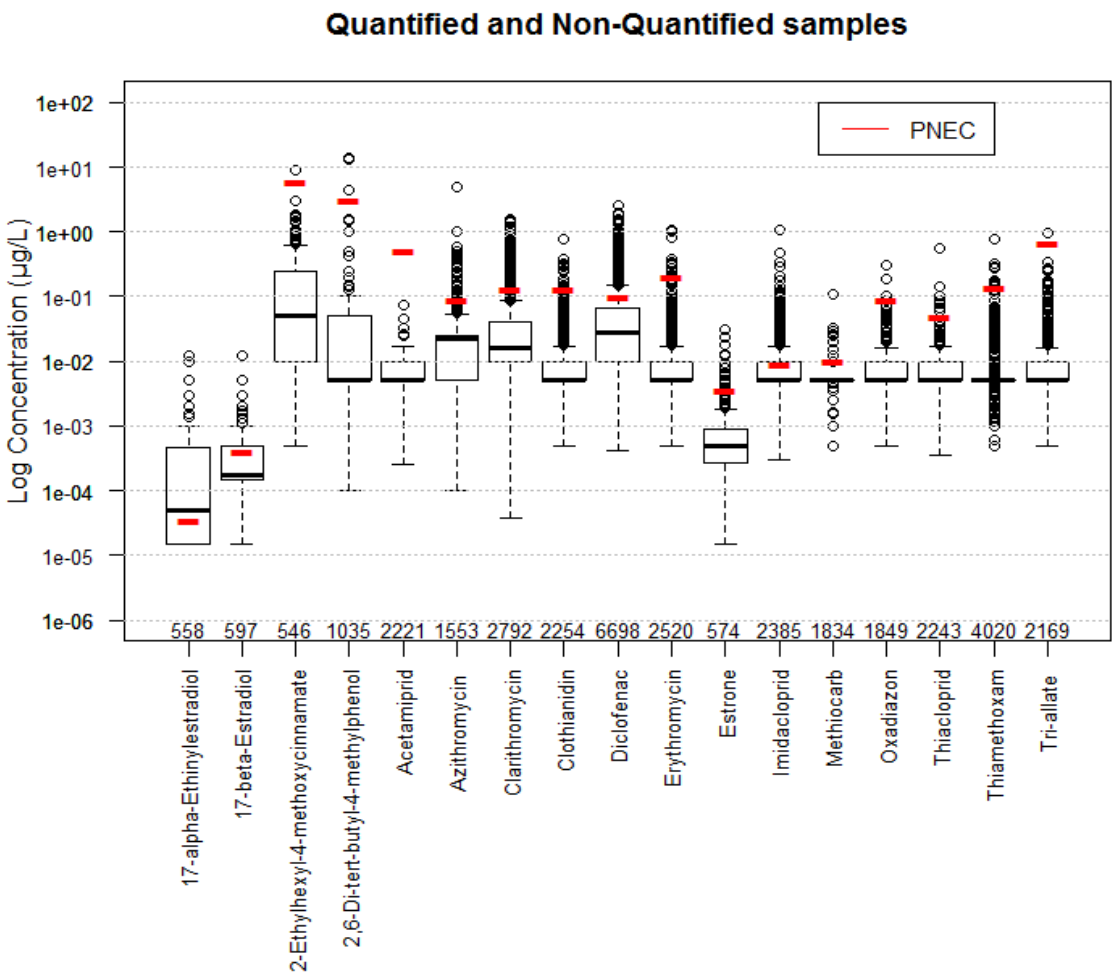
Annex 3.1 PNECs from 2015

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
17-alpha-Ethinylestradiol	3.50E-05	Sc2	25	223	558	476	14.70	1.50E-05	5.53E-04	1.80E-03	5.00E-05	1.00E-03	1.00E-03	1.25E-02
		Sc1	10	54	82	0	100.00	3.00E-05	2.28E-04	4.28E-04	1.00E-04	3.59E-04	7.79E-04	3.00E-03
		Sc3	14	122	323	241	25.39	1.50E-05	6.99E-05	2.34E-04	1.50E-05	1.51E-04	2.57E-04	3.00E-03
17-beta-Estradiol	4.00E-04	Sc2	25	228	597	496	16.92	1.50E-05	5.92E-04	1.72E-03	1.70E-04	7.00E-04	1.50E-03	1.25E-02
		Sc1	11	60	101	0	100.00	4.28E-05	4.11E-04	4.83E-04	2.10E-04	1.00E-03	1.30E-03	3.00E-03
		Sc3	18	180	462	361	21.86	1.50E-05	2.01E-04	2.56E-04	1.50E-04	2.50E-04	5.58E-04	3.00E-03
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Sc2	24	244	1035	978	5.51	1.00E-04	1.00E-01	6.66E-01	5.00E-03	1.05E-01	2.50E-01	1.40E+01
		Sc1	6	22	57	0	100.00	6.66E-03	5.12E-01	2.50E+00	1.80E-02	1.00E-01	2.60E-01	1.40E+01
		Sc3	23	241	1032	975	5.52	1.00E-04	8.77E-02	6.23E-01	5.00E-03	1.05E-01	2.50E-01	1.40E+01
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sc2	24	200	546	430	21.25	5.00E-04	3.67E-01	9.72E-01	5.00E-02	7.55E-01	3.00E+00	9.00E+00
		Sc1	6	19	116	0	100.00	3.00E-03	4.20E-01	4.05E-01	3.05E-01	1.00E+00	1.40E+00	1.80E+00
		Sc3	23	197	543	427	21.36	5.00E-04	3.19E-01	7.32E-01	5.00E-02	7.50E-01	3.00E+00	3.00E+00
Acetamiprid	5.00E-01	Sc2	24	372	2221	2206	0.68	2.50E-04	6.72E-03	6.17E-03	5.00E-03	1.00E-02	1.00E-02	7.40E-02
		Sc1	7	10	15	0	100.00	1.37E-03	1.41E-02	1.89E-02	9.00E-03	2.96E-02	4.46E-02	7.40E-02
		Sc3	24	372	2221	2206	0.68	2.50E-04	6.72E-03	6.17E-03	5.00E-03	1.00E-02	1.00E-02	7.40E-02
Azithromycin	9.00E-02	Sc2	24	288	1553	1288	17.06	1.00E-04	2.98E-02	1.85E-01	2.20E-02	3.29E-02	5.52E-02	5.00E+00
		Sc1	14	75	265	0	100.00	2.00E-04	6.16E-02	1.10E-01	2.30E-02	1.50E-01	2.49E-01	1.00E+00
		Sc3	24	286	1551	1286	17.09	1.00E-04	2.34E-02	4.96E-02	2.20E-02	3.20E-02	5.30E-02	1.00E+00
Clarithromycin	1.30E-01	Sc2	24	323	2792	1150	58.81	3.80E-05	4.71E-02	1.08E-01	1.60E-02	9.59E-02	1.74E-01	1.60E+00

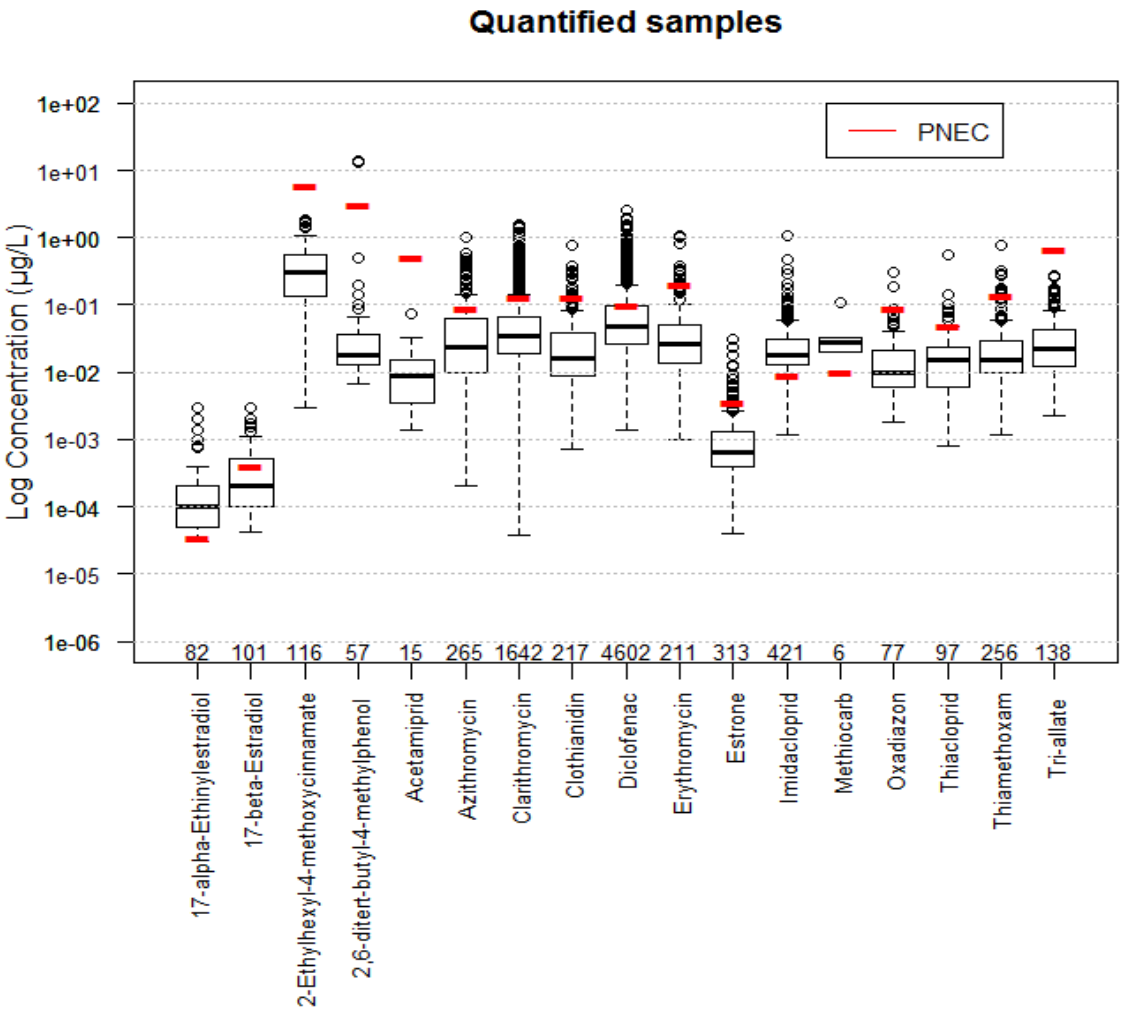
Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
		Sc1	17	201	1642	0	100.00	3.80E-05	7.33E-02	1.35E-01	3.40E-02	1.53E-01	2.80E-01	1.60E+00
		Sc3	24	323	2792	1150	58.81	3.80E-05	4.71E-02	1.08E-01	1.60E-02	9.59E-02	1.74E-01	1.60E+00
Clothianidin	1.30E-01	Sc2	24	343	2254	2037	9.63	5.00E-04	1.09E-02	2.77E-02	5.00E-03	1.10E-02	3.25E-02	7.80E-01
		Sc1	6	47	217	0	100.00	7.00E-04	4.35E-02	8.05E-02	1.60E-02	1.00E-01	1.73E-01	7.80E-01
		Sc3	24	343	2254	2037	9.63	5.00E-04	1.09E-02	2.77E-02	5.00E-03	1.10E-02	3.25E-02	7.80E-01
Diclofenac	1.00E-01	Sc2	25	607	6698	2096	68.71	4.25E-04	6.66E-02	1.26E-01	2.74E-02	1.60E-01	2.63E-01	2.60E+00
		Sc1	21	529	4602	0	100.00	1.40E-03	9.32E-02	1.45E-01	4.70E-02	2.10E-01	3.40E-01	2.60E+00
		Sc3	25	607	6698	2096	68.71	4.25E-04	6.66E-02	1.26E-01	2.74E-02	1.60E-01	2.63E-01	2.60E+00
Erythromycin	2.00E-01	Sc2	24	299	2520	2309	8.37	5.00E-04	1.15E-02	4.00E-02	5.00E-03	1.40E-02	2.81E-02	1.10E+00
		Sc1	12	89	211	0	100.00	1.00E-03	6.01E-02	1.27E-01	2.60E-02	1.00E-01	2.00E-01	1.10E+00
		Sc3	24	299	2520	2309	8.37	5.00E-04	1.15E-02	4.00E-02	5.00E-03	1.40E-02	2.81E-02	1.10E+00
Estrone	3.60E-03	Sc2	23	212	574	261	54.53	1.50E-05	1.29E-03	2.87E-03	5.00E-04	2.58E-03	5.00E-03	3.13E-02
		Sc1	13	141	313	0	100.00	3.97E-05	1.50E-03	3.14E-03	6.39E-04	2.99E-03	5.02E-03	3.13E-02
		Sc3	20	197	552	239	56.70	1.50E-05	1.01E-03	2.43E-03	5.00E-04	1.70E-03	3.50E-03	3.13E-02
Imidacloprid	9.00E-03	Sc2	24	376	2385	1964	17.65	3.00E-04	1.08E-02	2.83E-02	5.00E-03	1.70E-02	2.68E-02	1.05E+00
		Sc1	15	123	421	0	100.00	1.20E-03	3.12E-02	6.31E-02	1.80E-02	5.80E-02	8.20E-02	1.05E+00
		Sc3	22	326	1845	1424	22.82	3.00E-04	1.09E-02	3.21E-02	5.00E-03	2.00E-02	3.40E-02	1.05E+00
Methiocarb	1.00E-02	Sc2	24	369	1834	1828	0.33	5.00E-04	6.14E-03	4.10E-03	5.00E-03	1.00E-02	1.00E-02	1.09E-01
		Sc1	2	4	6	0	100.00	2.00E-02	3.96E-02	3.44E-02	2.79E-02	7.10E-02	9.00E-02	1.09E-01
		Sc3	22	356	1798	1792	0.33	5.00E-04	5.90E-03	3.66E-03	5.00E-03	1.00E-02	1.00E-02	1.09E-01
Oxadiazon	8.80E-02	Sc2	24	339	1849	1772	4.16	5.00E-04	1.10E-02	1.47E-02	5.00E-03	4.00E-02	4.00E-02	3.10E-01
		Sc1	5	17	77	0	100.00	1.80E-03	2.28E-02	4.25E-02	1.00E-02	5.00E-02	7.08E-02	3.10E-01
		Sc3	23	337	1847	1770	4.17	5.00E-04	1.09E-02	1.44E-02	5.00E-03	4.00E-02	4.00E-02	3.10E-01
Thiacloprid	5.00E-02	Sc2	24	374	2243	2146	4.32	3.50E-04	6.82E-03	1.35E-02	5.00E-03	1.00E-02	1.00E-02	5.70E-01
		Sc1	12	50	97	0	100.00	8.00E-04	2.64E-02	6.07E-02	1.50E-02	4.40E-02	7.90E-02	5.70E-01
		Sc3	24	374	2243	2146	4.32	3.50E-04	6.82E-03	1.35E-02	5.00E-03	1.00E-02	1.00E-02	5.70E-01

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
Thiamethoxam	1.40E-01	Sc2	24	418	4020	3764	6.37	5.00E-04	7.57E-03	1.81E-02	5.00E-03	1.00E-02	1.25E-02	7.70E-01
		Sc1	10	67	256	0	100.00	1.20E-03	3.16E-02	6.52E-02	1.50E-02	5.75E-02	1.23E-01	7.70E-01
		Sc3	24	418	4020	3764	6.37	5.00E-04	7.57E-03	1.81E-02	5.00E-03	1.00E-02	1.25E-02	7.70E-01
Tri-allate	6.70E-01	Sc2	24	338	2169	2031	6.36	5.00E-04	1.54E-02	4.50E-02	5.00E-03	2.50E-02	3.50E-02	9.45E-01
		Sc1	4	23	138	0	100.00	2.20E-03	3.73E-02	4.40E-02	2.20E-02	8.19E-02	1.13E-01	2.70E-01
		Sc3	23	335	2166	2028	6.37	5.00E-04	1.41E-02	2.89E-02	5.00E-03	2.50E-02	3.30E-02	3.35E-01

The figure below shows for Sc2 of WL dataset a box-whisker plot of all records (quantified and non-quantified) for WL substances in comparison to their PNEC values taken from the WL report 2015. The concentrations of the non-quantified samples are set to LOQ/2. The lowermost line of the figure also indicates the total number of samples per substance.



Next figure shows for Sc1 of WL dataset a box-whisker plot only of the quantified concentrations for WL substances in comparison to their PNEC according the WL report 2015. The figure also indicates the number of quantified samples per substance. Attention should be paid on the fact that for 2 substances (acetamiprid and methiocarb) the amount of the quantified samples is below the statistical threshold of 51 applied in the prioritisation monitoring exercise in 2016.


Quantified samples
PNEC
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
82 101 116 57 15 265 1642 217 4602 211 313 421 6 77 97 256 138
17-alpha-Ethinylestradiol
17-beta-Estradiol
2-Ethylhexyl-4-methoxycinnamate
2,6-ditert-butyl-4-methylphenol
Acetamiprid
Azithromycin
Clarithromycin
Clothianidin
Diclofenac
Erythromycin
Estrone
Imidacloprid
Methiocarb
Oxadiazon
Thiacloprid
Thiamethoxam
Tri-allate

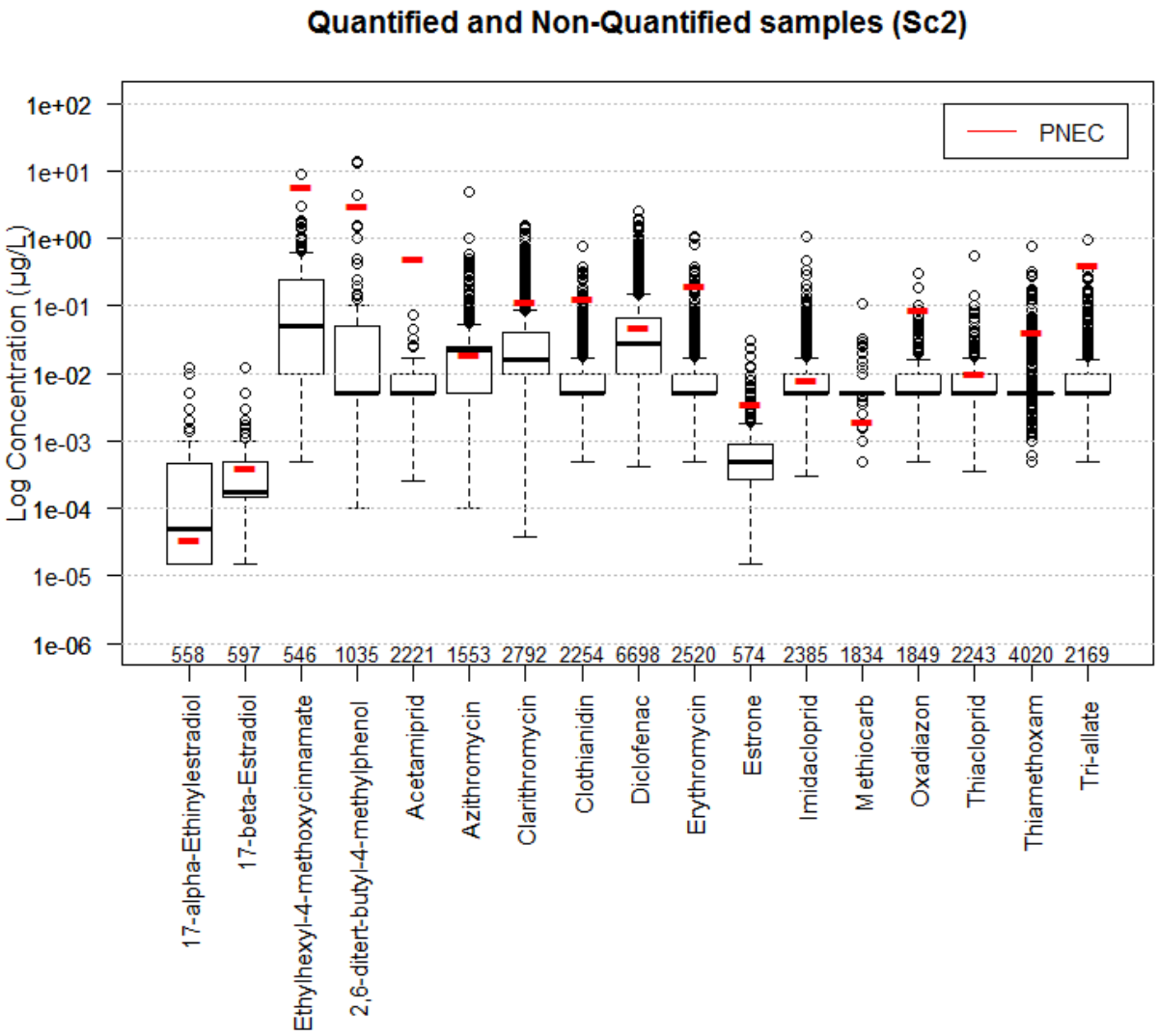
Annex 3.2 Updated PNECs

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
17-alpha-Ethinylestradiol	3.50E-05	Sc2	25	223	558	476	14.70	1.50E-05	5.53E-04	1.80E-03	5.00E-05	1.00E-03	1.00E-03	1.25E-02
		Sc1	10	54	82	0	100.00	3.00E-05	2.28E-04	4.28E-04	1.00E-04	3.59E-04	7.79E-04	3.00E-03
		Sc3	14	122	323	241	25.39	1.50E-05	6.99E-05	2.34E-04	1.50E-05	1.51E-04	2.57E-04	3.00E-03
17-beta-Estradiol	4.00E-04	Sc2	25	228	597	496	16.92	1.50E-05	5.92E-04	1.72E-03	1.70E-04	7.00E-04	1.50E-03	1.25E-02
		Sc1	11	60	101	0	100.00	4.28E-05	4.11E-04	4.83E-04	2.10E-04	1.00E-03	1.30E-03	3.00E-03
		Sc3	18	180	462	361	21.86	1.50E-05	2.01E-04	2.56E-04	1.50E-04	2.50E-04	5.58E-04	3.00E-03
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Sc2	24	244	1035	978	5.51	1.00E-04	1.00E-01	6.66E-01	5.00E-03	1.05E-01	2.50E-01	1.40E+01
		Sc1	6	22	57	0	100.00	6.66E-03	5.12E-01	2.50E+00	1.80E-02	1.00E-01	2.60E-01	1.40E+01
		Sc3	23	241	1032	975	5.52	1.00E-04	8.77E-02	6.23E-01	5.00E-03	1.05E-01	2.50E-01	1.40E+01
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sc2	24	200	546	430	21.25	5.00E-04	3.67E-01	9.72E-01	5.00E-02	7.55E-01	3.00E+00	9.00E+00
		Sc1	6	19	116	0	100.00	3.00E-03	4.20E-01	4.05E-01	3.05E-01	1.00E+00	1.40E+00	1.80E+00
		Sc3	23	197	543	427	21.36	5.00E-04	3.19E-01	7.32E-01	5.00E-02	7.50E-01	3.00E+00	3.00E+00
Acetamiprid	5.00E-01	Sc2	24	372	2221	2206	0.68	2.50E-04	6.72E-03	6.17E-03	5.00E-03	1.00E-02	1.00E-02	7.40E-02
		Sc1	7	10	15	0	100.00	1.37E-03	1.41E-02	1.89E-02	9.00E-03	2.96E-02	4.46E-02	7.40E-02
		Sc3	24	372	2221	2206	0.68	2.50E-04	6.72E-03	6.17E-03	5.00E-03	1.00E-02	1.00E-02	7.40E-02
Azithromycin	1.90E-02	Sc2	24	288	1553	1288	17.06	1.00E-04	2.98E-02	1.85E-01	2.20E-02	3.29E-02	5.52E-02	5.00E+00
		Sc1	14	75	265	0	100.00	2.00E-04	6.16E-02	1.10E-01	2.30E-02	1.50E-01	2.49E-01	1.00E+00
		Sc3	19	192	915	650	28.96	1.00E-04	2.14E-02	6.43E-02	5.00E-03	4.59E-02	8.53E-02	1.00E+00
Clarithromycin	1.20E-01	Sc2	24	323	2792	1150	58.81	3.80E-05	4.71E-02	1.08E-01	1.60E-02	9.59E-02	1.74E-01	1.60E+00

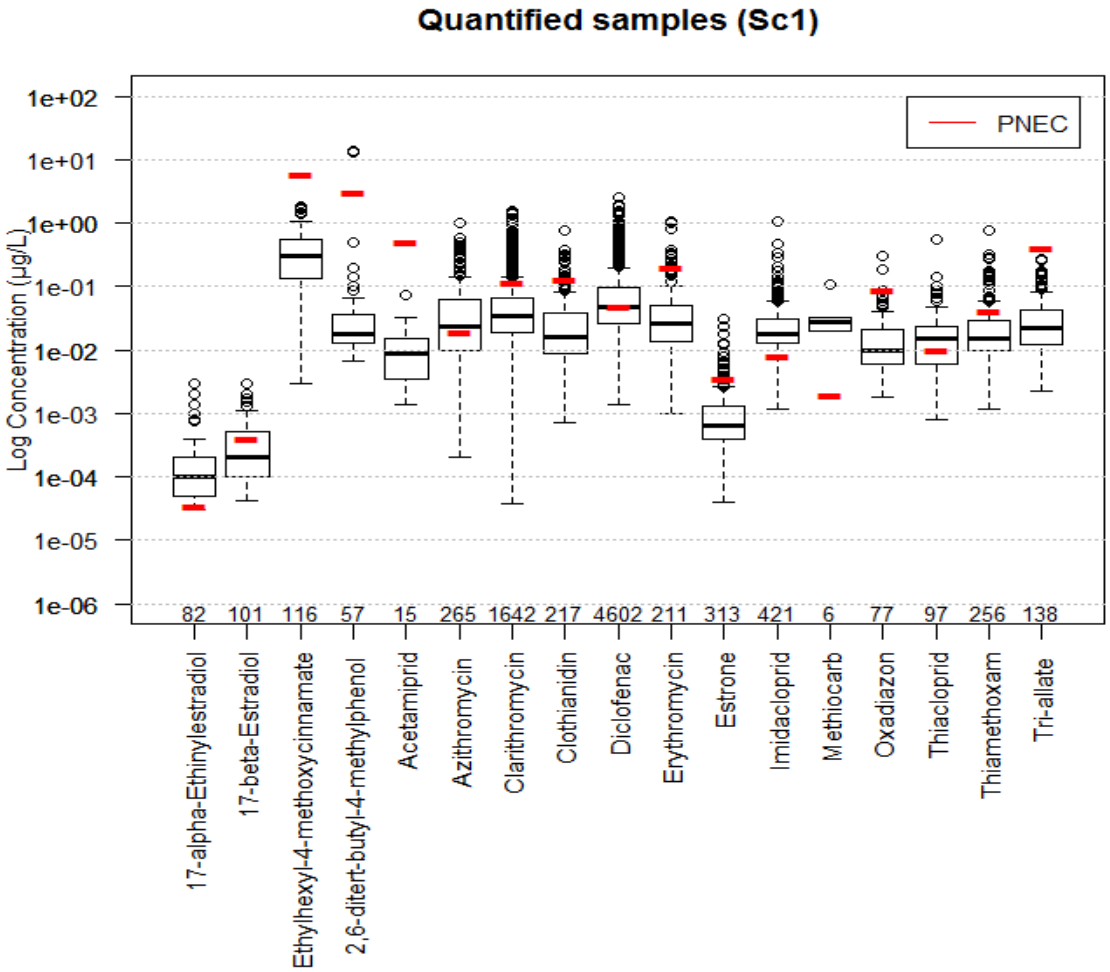
Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
		Sc1	17	201	1642	0	100.00	3.80E-05	7.33E-02	1.35E-01	3.40E-02	1.53E-01	2.80E-01	1.60E+00
		Sc3	24	323	2792	1150	58.81	3.80E-05	4.71E-02	1.08E-01	1.60E-02	9.59E-02	1.74E-01	1.60E+00
Clothianidin	1.30E-01	Sc2	24	343	2254	2037	9.63	5.00E-04	1.09E-02	2.77E-02	5.00E-03	1.10E-02	3.25E-02	7.80E-01
		Sc1	6	47	217	0	100.00	7.00E-04	4.35E-02	8.05E-02	1.60E-02	1.00E-01	1.73E-01	7.80E-01
		Sc3	24	343	2254	2037	9.63	5.00E-04	1.09E-02	2.77E-02	5.00E-03	1.10E-02	3.25E-02	7.80E-01
Diclofenac	5.00E-02	Sc2	25	607	6698	2096	68.71	4.25E-04	6.66E-02	1.26E-01	2.74E-02	1.60E-01	2.63E-01	2.60E+00
		Sc1	21	529	4602	0	100.00	1.40E-03	9.32E-02	1.45E-01	4.70E-02	2.10E-01	3.40E-01	2.60E+00
		Sc3	25	607	6698	2096	68.71	4.25E-04	6.66E-02	1.26E-01	2.74E-02	1.60E-01	2.63E-01	2.60E+00
Erythromycin	2.00E-01	Sc2	24	300	2520	2309	8.37	5.00E-04	1.15E-02	4.00E-02	5.00E-03	1.40E-02	2.81E-02	1.10E+00
		Sc1	12	89	211	0	100.00	1.00E-03	6.01E-02	1.27E-01	2.60E-02	1.00E-01	2.00E-01	1.10E+00
		Sc3	24	300	2520	2309	8.37	5.00E-04	1.15E-02	4.00E-02	5.00E-03	1.40E-02	2.81E-02	1.10E+00
Estrone	3.60E-03	Sc2	23	212	574	261	54.53	1.50E-05	1.29E-03	2.87E-03	5.00E-04	2.58E-03	5.00E-03	3.13E-02
		Sc1	13	141	313	0	100.00	3.97E-05	1.50E-03	3.14E-03	6.39E-04	2.99E-03	5.02E-03	3.13E-02
		Sc3	20	197	552	239	56.70	1.50E-05	1.01E-03	2.43E-03	5.00E-04	1.70E-03	3.50E-03	3.13E-02
Imidacloprid	8.30E-03	Sc2	24	376	2385	1964	17.65	3.00E-04	1.08E-02	2.83E-02	5.00E-03	1.70E-02	2.68E-02	1.05E+00
		Sc1	15	123	421	0	100.00	1.20E-03	3.12E-02	6.31E-02	1.80E-02	5.80E-02	8.20E-02	1.05E+00
		Sc3	22	326	1845	1424	22.82	3.00E-04	1.09E-02	3.21E-02	5.00E-03	2.00E-02	3.40E-02	1.05E+00
Methiocarb	2.00E-03	Sc2	24	369	1834	1828	0.33	5.00E-04	6.14E-03	4.10E-03	5.00E-03	1.00E-02	1.00E-02	1.09E-01
		Sc1	2	4	6	0	100.00	2.00E-02	3.96E-02	3.44E-02	2.79E-02	7.10E-02	9.00E-02	1.09E-01
		Sc3	7	56	127	121	4.72	5.00E-04	2.76E-03	1.07E-02	1.00E-03	1.50E-03	1.65E-03	1.09E-01
Oxadiazon	8.80E-02	Sc2	24	339	1849	1772	4.16	5.00E-04	1.10E-02	1.47E-02	5.00E-03	4.00E-02	4.00E-02	3.10E-01
		Sc1	5	17	77	0	100.00	1.80E-03	2.28E-02	4.25E-02	1.00E-02	5.00E-02	7.08E-02	3.10E-01
		Sc3	23	337	1847	1770	4.17	5.00E-04	1.09E-02	1.44E-02	5.00E-03	4.00E-02	4.00E-02	3.10E-01

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
Thiacloprid	1.00E-02	Sc2	24	374	2243	2146	4.32	3.50E-04	6.82E-03	1.35E-02	5.00E-03	1.00E-02	1.00E-02	5.70E-01
		Sc1	12	50	97	0	100.00	8.00E-04	2.64E-02	6.07E-02	1.50E-02	4.40E-02	7.90E-02	5.70E-01
		Sc3	23	366	2235	2138	4.34	3.50E-04	6.79E-03	1.35E-02	5.00E-03	1.00E-02	1.00E-02	5.70E-01
Thiamethoxam	4.20E-02	Sc2	24	418	4020	3764	6.37	5.00E-04	7.57E-03	1.81E-02	5.00E-03	1.00E-02	1.25E-02	7.70E-01
		Sc1	10	67	256	0	100.00	1.20E-03	3.16E-02	6.52E-02	1.50E-02	5.75E-02	1.23E-01	7.70E-01
		Sc3	23	412	3979	3723	6.43	5.00E-04	7.18E-03	1.78E-02	5.00E-03	1.00E-02	1.00E-02	7.70E-01
Tri-allate	4.10E-01	Sc2	24	338	2169	2031	6.36	5.00E-04	1.54E-02	4.50E-02	5.00E-03	2.50E-02	3.50E-02	9.45E-01
		Sc1	4	23	138	0	100.00	2.20E-03	3.73E-02	4.40E-02	2.20E-02	8.19E-02	1.13E-01	2.70E-01
		Sc3	23	335	2166	2028	6.37	5.00E-04	1.41E-02	2.89E-02	5.00E-03	2.50E-02	3.30E-02	3.35E-01

The figure below shows for Sc2 of WL dataset a box-whisker plot of all records (quantified and non-quantified) for WL substances in comparison to the updated PNECs. The concentrations of the non-quantified samples are set to LOQ/2. The lowermost line of the figure also indicates the total number of samples per substance.


Quantified and Non-Quantified samples (Sc2)
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
PNEC
558
597
546
1035
2221
1553
2792
2254
6698
2520
574
2385
1834
1849
2243
4020
2169
17-alpha-Ethinylestradiol
17-beta-Estradiol
Ethylhexyl-4-methoxycinnamate
2,6-ditert-butyl-4-methylphenol
Acetamiprid
Azithromycin
Clarithromycin
Clothianidin
Diclofenac
Erythromycin
Estrone
Imidacloprid
Methiocarb
Oxadiazon
Thiacloprid
Thiamethoxam
Tri-allate

The next figure presents for Sc1 of WL dataset a box-whisker plot only of the quantified concentrations for WL substances in comparison to the updated PNECs. The figure also indicates the number of quantified samples per substance. Attention should be paid on the fact that for 2 substances (acetamiprid and methiocarb) the amount of the quantified samples is below the statistical threshold of 51 applied in the prioritisation monitoring exercise in 2016.



Annex 4: Analysis on LOQs by WL dataset for non-quantified samples of substances with reduced data quality (Sc2)

Annex 4.1. EE2 (PNEC = 0.000035 µg/L).

LOQ (µg/L)	# of samples	Countries (#)
0.000030	172	3, 7, 13, 26
0.000035	57	11, 19, 20, 22
0.00005	11	6, 7
0.00006	1	13
0.0001	70	1, 2, 6, 7, 12, 24
0.00013	1	7
0.00025	3	7
0.0003	11	5, 7
0.0004	16	16, 27
0.00094	2	15
0.001	24	6, 8, 19, 29, 31
0.002	88	6, 8, 28
0.003	1	8
0.01	8	9, 21
0.02	1	8
0.025	10	30

Annex 4.2. E2 (PNEC = 0.0004 µg/L).

LOQ (µg/L)	# of samples	Countries (#)
0.00003	16	7, 13
0.00005	1	7
0.0001	44	1, 7, 19, 24
0.00012	8	7
0.0002	7	7
0.00025	17	7
0.0003	163	6, 26
0.0004	104	2, 3, 7, 9, 11, 12, 16, 19, 20, 22, 27
0.0005	2	7
0.00099	2	15
0.001	88	6, 8, 29

0.0012	3	5
0.002	3	2, 8
0.003	17	8, 28
0.01	12	9, 21, 31
0.025	10	30

Annex 4.3. Estrone (PNEC = 0.0036 µg/L).

LOQ (µg/L)	# of samples	Countries (#)
0.00003	1	7
0.0001	9	19, 24
0.0003	33	26
0.0004	50	2, 7, 11, 12, 16, 19, 20, 22
0.0005	14	7
0.00087	2	15
0.0009	3	5
0.001	122	6, 8, 29
0.002	4	2, 8
0.0025	2	2
0.003	1	8
0.01	12	9, 21, 31
0.025	10	30

Annex 4.4. Imidacloprid (PNEC = 0.009 µg/L).

LOQ (µg/L)	# of samples	Countries (#)
0.0006	1	7
0.001	18	2, 7, 13, 17
0.0012	7	15
0.005	47	7, 9, 11, 19
0.006	11	24
0.009	123	3, 5, 7, 16, 19, 20, 22, 31
0.01	1070	2, 6, 7, 9, 12, 19, 29, 30
0.011	109	26
0.013	38	1
0.02	519	6, 7, 19, 21, 29

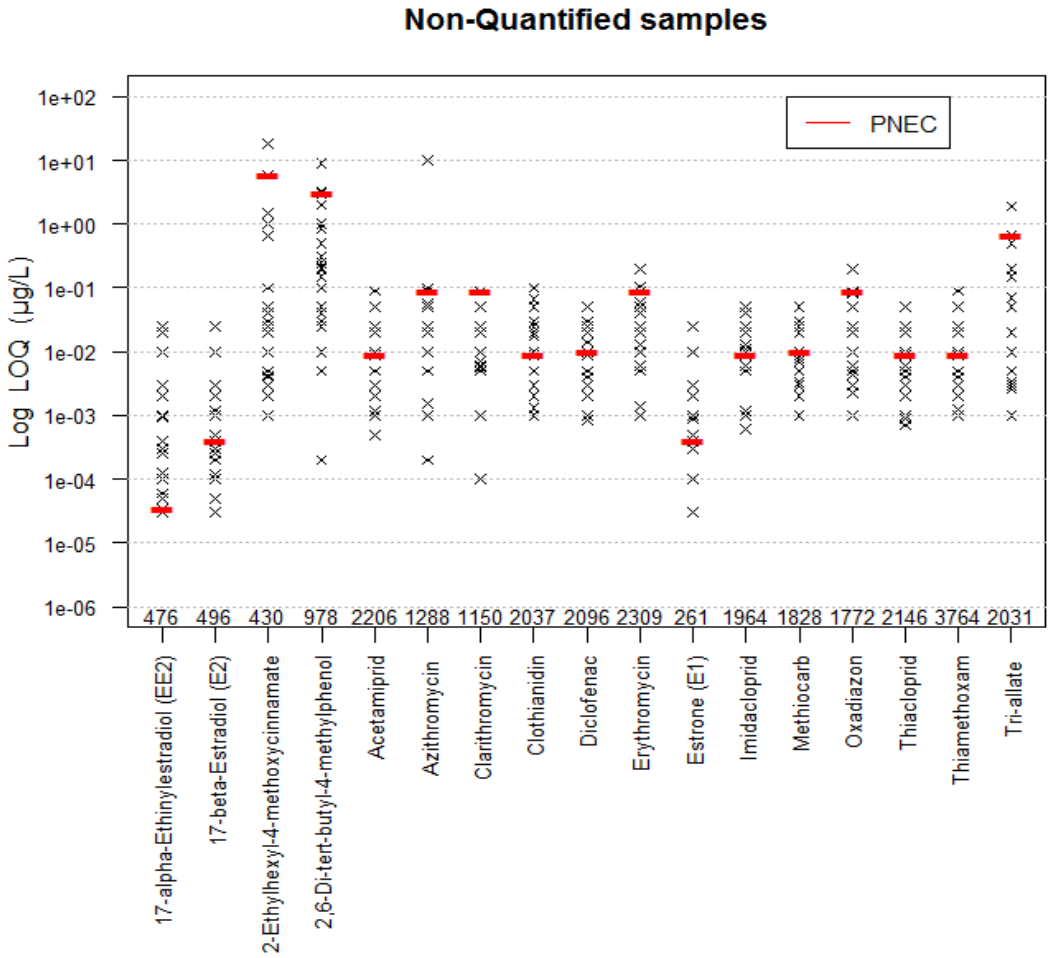
0.025	5	27
0.04	1	29
0.05	15	8, 9, 29

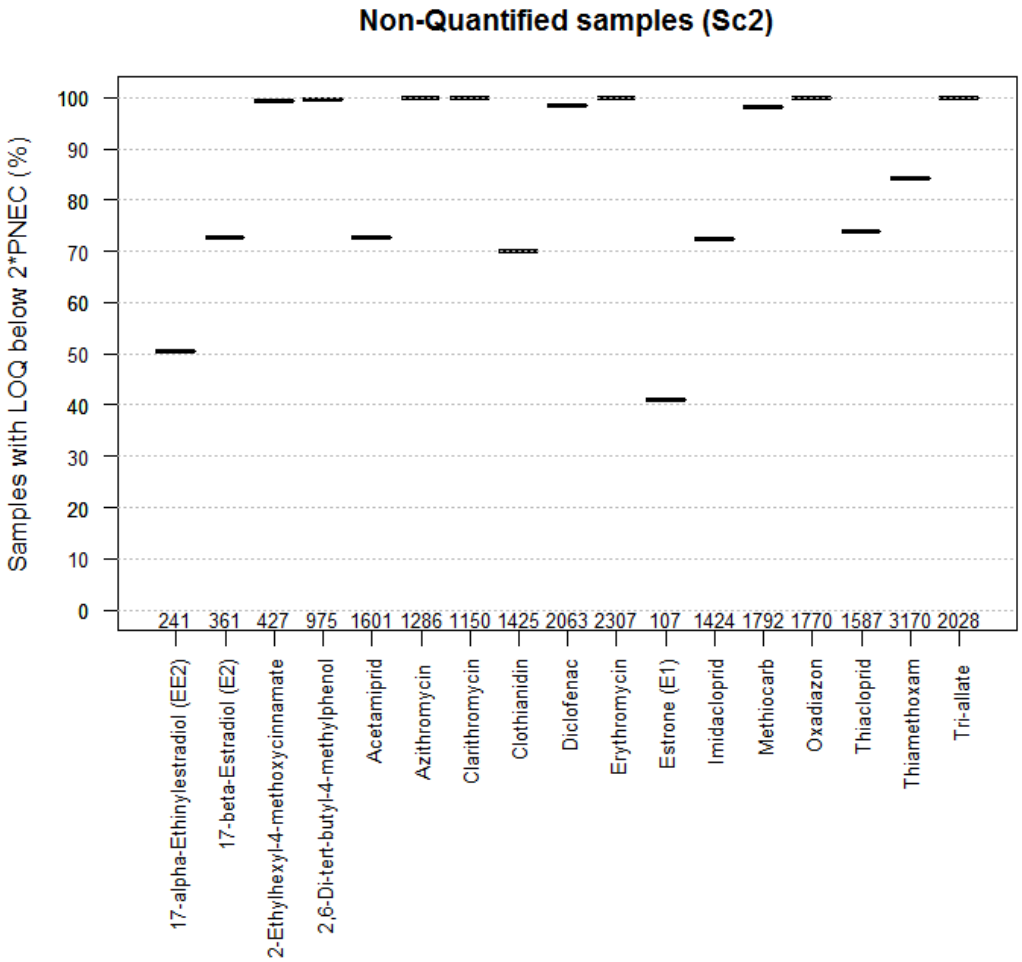
Annex 4.5. Methiocarb (PNEC = 0.01 µg/L).

LOQ (µg/L)	# of samples	Countries (#)
0.001	29	13, 17
0.002	81	29
0.003	8	7
0.0033	3	15
0.005	26	6, 7, 9, 11
0.007	12	7
0.008	41	1
0.009	10	16
0.01	1176	2, 3, 5, 6, 7, 9, 12, 19, 20, 24, 30, 31
0.02	406	2, 6, 7, 8, 9, 26
0.025	16	7, 27
0.03	4	21
0.05	16	7

Annex 4.6. Data quality check versus the maximum acceptable method detection limit (Decision EU/2015/495)

On the figures shown below PNEC values are considered as equal to the maximum acceptable method detection limit (Commission Implementing Decision EU/2015/495).





The WL data quality check according to the maximum acceptable method detection limit (Commission Implementing Decision EU/2015/495) allows concluding that all Estrogens and Neonicotinoid insecticides have a reduced but adequate data quality to perform a relevant assessment.

Annex 5: STE results by the WL dataset

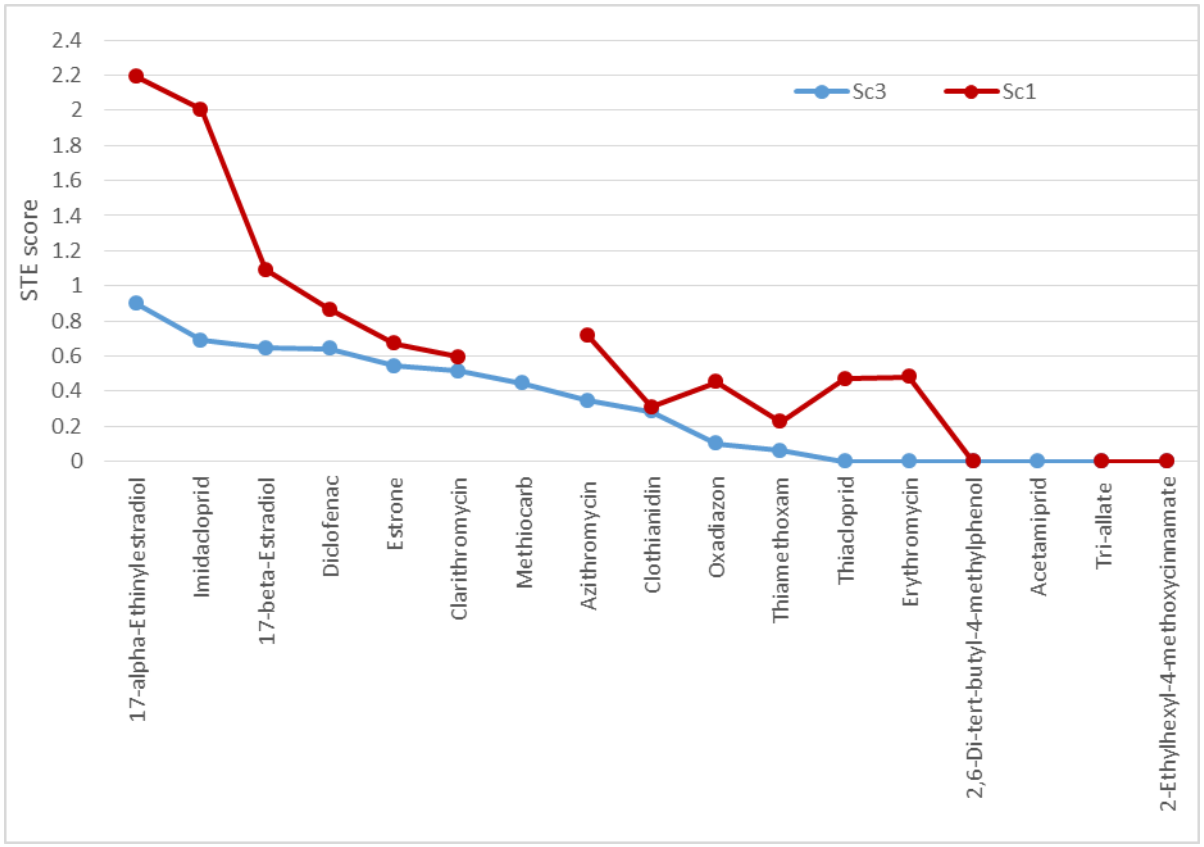
Annex 5.1 PNECs from 2015: STE factors, STE scores and RQ(P95) for all data scenarios.

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
57-63-6	17-alpha-Ethinylestradiol	3.50E-05	Estrogen	Sc2	2.86E+01	5.66E-01	7.84E-01	5.60E-01	1.91E+00
				Sc1	2.23E+01	9.26E-01	9.85E-01	2.80E-01	2.19E+00
				Sc3	7.35E+00	2.67E-01	5.21E-01	1.10E-01	8.99E-01
50-28-2	17-beta-Estradiol	4.00E-04	Estrogen	Sc2	3.75E+00	2.01E-01	7.84E-01	1.80E-01	1.17E+00
				Sc1	3.26E+00	3.00E-01	7.20E-01	7.00E-02	1.09E+00
				Sc3	1.28E+00	5.40E-02	5.58E-01	7.00E-02	6.82E-01
128-37-0	2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	Sc2	7.91E-02	6.80E-04	1.67E-01	0.00E+00	1.67E-01
				Sc1	8.23E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	7.91E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5466-77-3	2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	Sc2	5.00E-01	6.22E-04	0.00E+00	0.00E+00	6.22E-04
				Sc1	2.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
135410-20-7	Acetamiprid	5.00E-01	Neonicotinoid Insecticide	Sc2	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	8.92E-02	n/a	n/a	n/a	n/a
				Sc3	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
83905-01-5	Azithromycin	9.00E-02	Antibiotic	Sc2	6.13E-01	7.81E-03	3.03E-01	4.00E-02	3.51E-01
				Sc1	2.77E+00	1.09E-01	5.42E-01	7.00E-02	7.20E-01
				Sc3	5.89E-01	4.66E-03	3.03E-01	4.00E-02	3.48E-01
81103-11-9	Clarithromycin	1.30E-01	Antibiotic	Sc2	1.34E+00	2.57E-02	4.19E-01	7.00E-02	5.15E-01
				Sc1	2.15E+00	8.19E-02	4.41E-01	7.00E-02	5.93E-01
				Sc3	1.34E+00	2.57E-02	4.19E-01	7.00E-02	5.15E-01

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
210880-92-5	Clothianidin	1.30E-01	Neonicotinoid Insecticide	Sc2	2.50E-01	2.43E-04	2.85E-01	0.00E+00	2.86E-01
				Sc1	1.33E+00	2.13E-02	2.48E-01	4.00E-02	3.09E-01
				Sc3	2.50E-01	2.43E-04	2.85E-01	0.00E+00	2.86E-01
15307-86-5	Diclofenac	1.00E-01	Analgesic	Sc2	2.63E+00	2.10E-01	3.65E-01	7.00E-02	6.45E-01
				Sc1	3.40E+00	3.12E-01	4.42E-01	1.10E-01	8.64E-01
				Sc3	2.63E+00	2.10E-01	3.65E-01	7.00E-02	6.45E-01
114-07-8	Erythromycin	2.00E-01	Antibiotic	Sc2	1.41E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	1.00E+00	1.31E-02	4.27E-01	4.00E-02	4.80E-01
				Sc3	1.41E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
53-16-7	Estrone	3.60E-03	Estrogen	Sc2	1.39E+00	6.12E-02	6.65E-01	7.00E-02	7.96E-01
				Sc1	1.39E+00	6.11E-02	5.71E-01	4.00E-02	6.72E-01
				Sc3	9.72E-01	2.12E-02	4.81E-01	4.00E-02	5.42E-01
138261-41-3	Imidacloprid	9.00E-03	Neonicotinoid Insecticide	Sc2	2.98E+00	2.77E-01	6.21E-01	1.10E-01	1.01E+00
				Sc1	9.11E+00	8.42E-01	9.83E-01	1.80E-01	2.00E+00
				Sc3	3.67E+00	1.87E-01	4.34E-01	1.10E-01	7.31E-01
2032-65-7	Methiocarb	1.00E-02	Insecticide/Herbicide	Sc2	1.00E+00	7.68E-03	8.60E-01	4.00E-02	9.08E-01
				Sc1	9.00E+00	n/a	n/a	n/a	n/a
				Sc3	1.00E+00	5.11E-04	4.05E-01	4.00E-02	4.45E-01
19666-30-9	Oxadiazon	8.80E-02	Herbicide	Sc2	4.55E-01	9.83E-04	1.00E-01	0.00E+00	1.01E-01
				Sc1	8.05E-01	4.71E-02	3.33E-01	7.00E-02	4.50E-01
				Sc3	4.55E-01	2.58E-04	1.00E-01	0.00E+00	1.00E-01
111988-49-9	Thiacloprid	5.00E-02	Neonicotinoid Insecticide	Sc2	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	1.58E+00	5.33E-02	3.45E-01	7.00E-02	4.69E-01
				Sc3	2.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
153719-23-4	Thiamethoxam	1.40E-01	Neonicotinoid Insecticide	Sc2	8.93E-02	9.97E-05	6.14E-02	0.00E+00	6.15E-02
				Sc1	8.75E-01	4.48E-03	2.23E-01	0.00E+00	2.27E-01
				Sc3	8.93E-02	9.97E-05	6.14E-02	0.00E+00	6.15E-02
2303-17-5	Tri-allate	6.70E-01	Herbicide	Sc2	5.22E-02	3.70E-04	0.00E+00	0.00E+00	3.70E-04
				Sc1	1.69E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	4.93E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00

The figure shows a comparison of STE scores obtained by WL dataset for scenarios Sc1 and Sc3. In Sc1 no scores were presented for methiocarb and acetamiprid since they did not fulfil the representativity criteria for this scenario. PNECs correspond to those in the WL report 2015.



The table below gives per substance for Sc3 and PNECs from 2005 information for the site (Fs,site) and country (Fs,country) frequency of exceedances in Fspat, the calculation of Ftemp by all sites (Ftemp_1) and excluding sites with a single measurement that exceeds PNEC (Ftemp_2), the size of the exceedance extent in Fext, the percentage (from the total number of samples) of samples that exceed PNEC and the total amount of samples.

Substance	PNEC (µg/L) (WL report 2015)	Type	Fs,site	Fs,country	Ftemp_1	Ftemp_2	EXCextent	Exceeding samples (%)	Number of samples (Sc3)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	3.74E-01	7.14E-01	7.13E-01	5.21E-01	9.79E+00	22.91	323
17-beta-Estradiol	4.00E-04	Estrogen	1.17E-01	4.12E-01	7.26E-01	5.58E-01	1.87E+00	6.72	461
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	4.13E-03	0.00E+00	1.67E-01	1.67E-01	3.09E-01	0.19	1032
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.00E-01	0.00	543
Acetamiprid	5.00E-01	Neonicotinoid Insecticide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.50E-02	0.00	2221
Azithromycin	9.00E-02	Antibiotic	5.59E-02	8.33E-02	3.40E-01	3.03E-01	1.13E+00	2.71	1551
Clarithromycin	1.30E-01	Antibiotic	1.23E-01	2.08E-01	4.19E-01	4.06E-01	2.29E+00	7.02	2792
Clothianidin	1.30E-01	Neonicotinoid Insecticide	5.83E-03	4.17E-02	2.85E-01	2.85E-01	2.50E-01	0.67	2254
Diclofenac	1.00E-01	Analgesic	3.49E-01	6.00E-01	3.64E-01	3.29E-01	4.39E+00	16.11	6697
Erythromycin	2.00E-01	Antibiotic	1.33E-02	0.00E+00	2.68E-01	1.46E-01	4.25E-01	0.44	2520
Estrone	3.60E-03	Estrogen	7.07E-02	3.00E-01	6.75E-01	4.81E-01	1.30E+00	4.53	552
Imidacloprid	9.00E-03	Neonicotinoid Insecticide	3.02E-01	5.45E-01	5.53E-01	4.16E-01	6.61E+00	19.29	1830
Methiocarb	1.00E-02	Insecticide/Herbicide	1.12E-02	4.55E-02	4.05E-01	4.05E-01	1.00E+00	0.33	1798
Oxadiazon	8.80E-02	Herbicide	5.93E-03	4.35E-02	5.50E-01	1.00E-01	5.00E-01	0.11	1847
Thiacloprid	5.00E-02	Neonicotinoid Insecticide	1.07E-02	0.00E+00	9.76E-02	9.76E-02	3.60E-01	0.36	2243
Thiamethoxam	1.40E-01	Neonicotinoid Insecticide	2.39E-03	4.17E-02	6.14E-02	6.14E-02	2.01E-01	0.25	4020
Triallate	6.70E-01	Herbicide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-01	0.00	2166

Annex 5.2 WL data and updated PNECs: STE factors, STE scores and RQ(P95) for all scenarios.

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
57-63-6	17-alpha-Ethinylestradiol	3.50E-05	Estrogen	Sc2	2.86E+01	5.66E-01	7.84E-01	5.60E-01	1.91E+00
				Sc1	2.23E+01	9.26E-01	9.85E-01	2.80E-01	2.19E+00
				Sc3	7.35E+00	2.67E-01	5.21E-01	1.10E-01	8.99E-01
50-28-2	17-beta-Estradiol	4.00E-04	Estrogen	Sc2	3.75E+00	2.01E-01	7.84E-01	1.80E-01	1.17E+00
				Sc1	3.26E+00	3.00E-01	7.20E-01	7.00E-02	1.09E+00
				Sc3	1.40E+00	5.40E-02	5.58E-01	7.00E-02	6.82E-01
128-37-0	2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	Sc2	7.91E-02	6.80E-04	1.67E-01	0.00E+00	1.67E-01
				Sc1	8.23E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	7.91E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5466-77-3	2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	Sc2	5.00E-01	6.22E-04	0.00E+00	0.00E+00	6.22E-04
				Sc1	2.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
135410-20-7	Acetamiprid	5.00E-01	Neonicotinoid Insecticide	Sc2	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	8.92E-02	n/a	n/a	n/a	n/a
				Sc3	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
83905-01-5	Azithromycin	1.90E-02	Antibiotic	Sc2	2.91E+00	3.96E-01	8.97E-01	1.10E-01	1.40E+00
				Sc1	1.31E+01	5.45E-01	7.45E-01	2.80E-01	1.57E+00
				Sc3	4.49E+00	1.45E-01	6.24E-01	1.10E-01	8.79E-01

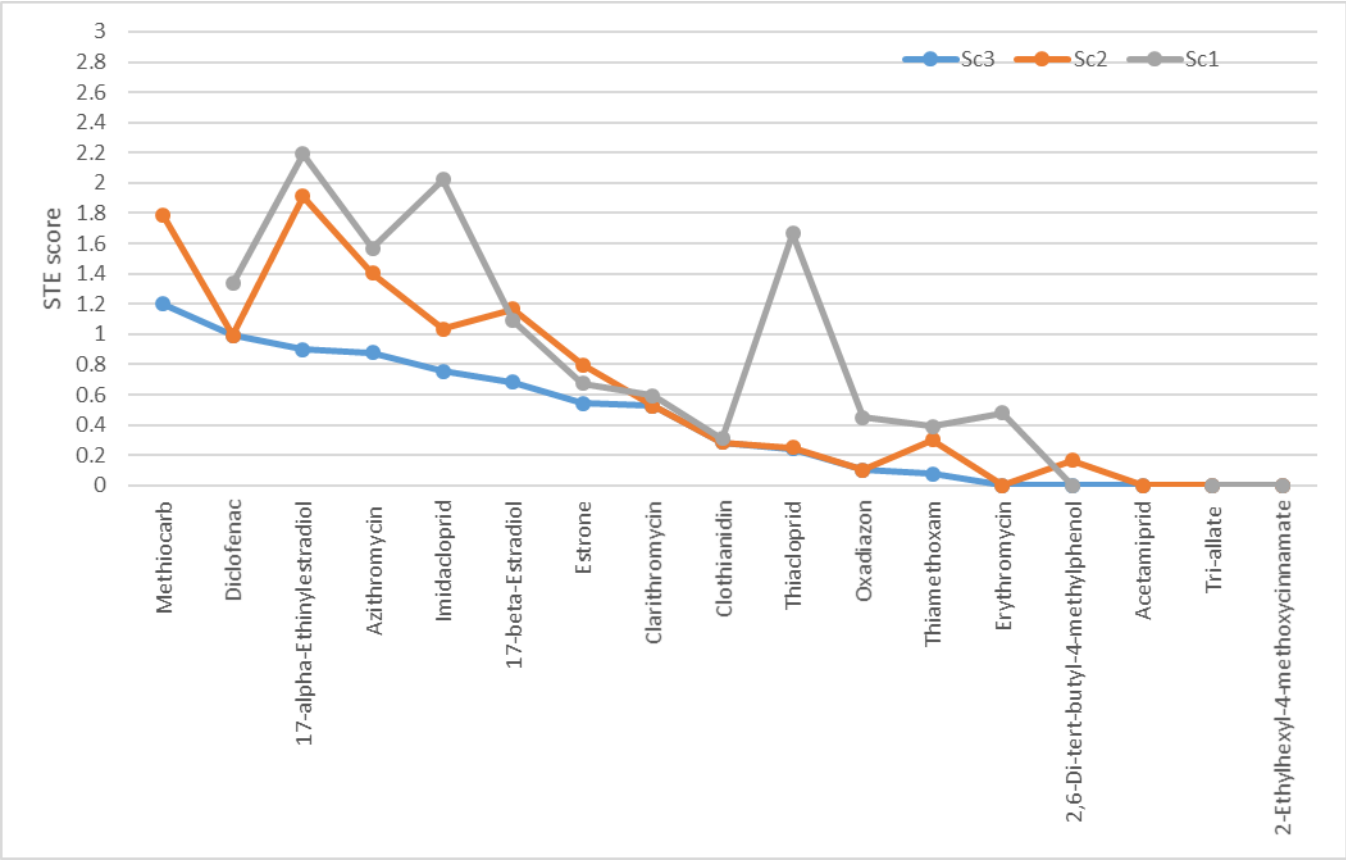
CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
81103-11-9	Clarithromycin	1.20E-01	Antibiotic	Sc2	1.45E+00	2.83E-02	4.27E-01	7.00E-02	5.25E-01
				Sc1	2.33E+00	9.01E-02	4.35E-01	7.00E-02	5.95E-01
				Sc3	1.45E+00	2.83E-02	4.27E-01	7.00E-02	5.25E-01
210880-92-5	Clothianidin	1.30E-01	Neonicotinoid Insecticide	Sc2	2.50E-01	2.43E-04	2.85E-01	0.00E+00	2.86E-01
				Sc1	1.33E+00	2.13E-02	2.48E-01	4.00E-02	3.09E-01
				Sc3	2.50E-01	2.43E-04	2.85E-01	0.00E+00	2.86E-01
15307-86-5	Diclofenac	5.00E-02	Analgesic	Sc2	5.26E+00	4.05E-01	4.75E-01	1.10E-01	9.90E-01
				Sc1	6.80E+00	5.75E-01	5.80E-01	1.80E-01	1.34E+00
				Sc3	5.26E+00	4.05E-01	4.75E-01	1.10E-01	9.90E-01
114-07-8	Erythromycin	2.00E-01	Antibiotic	Sc2	1.41E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	1.00E+00	1.31E-02	4.27E-01	4.00E-02	4.80E-01
				Sc3	1.41E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
53-16-7	Estrone	3.60E-03	Estrogen	Sc2	1.39E+00	6.12E-02	6.65E-01	7.00E-02	7.96E-01
				Sc1	1.39E+00	6.11E-02	5.71E-01	4.00E-02	6.72E-01
				Sc3	9.72E-01	2.12E-02	4.81E-01	4.00E-02	5.42E-01
138261-41-3	Imidacloprid	8.30E-03	Neonicotinoid Insecticide	Sc2	3.23E+00	3.03E-01	6.19E-01	1.10E-01	1.03E+00
				Sc1	9.88E+00	8.57E-01	9.84E-01	1.80E-01	2.02E+00
				Sc3	4.10E+00	2.09E-01	4.35E-01	1.10E-01	7.53E-01
2032-65-7	Methiocarb	2.00E-03	Insecticide/Herbicide	Sc2	5.00E+00	7.16E-01	1.00E+00	7.00E-02	1.79E+00
				Sc1	4.50E+01	n/a	n/a	n/a	n/a
				Sc3	8.25E+01	2.04E-02	1.00E-00	1.80E-01	1.20E+00
19666-30-9	Oxadiazon	8.80E-02	Herbicide	Sc2	4.55E-01	9.83E-04	1.00E-01	0.00E+00	1.01E-01

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
				Sc1	8.05E-01	4.71E-02	3.33E-01	7.00E-02	4.50E-01
				Sc3	4.55E-01	2.58E-04	1.00E-01	0.00E+00	1.00E-01
111988-49-9	Thiacloprid	1.00E-02	Neonicotinoid Insecticide	Sc2	1.00E+00	2.12E-02	1.89E-01	4.00E-02	2.51E-01
				Sc1	7.90E+00	5.55E-01	9.31E-01	1.80E-01	1.67E+00
				Sc3	1.00E+00	1.07E-02	1.89E-01	4.00E-02	2.40E-01
153719-23-4	Thiamethoxam	4.20E-02	Neonicotinoid Insecticide	Sc2	2.98E-01	2.19E-03	2.98E-01	0.00E+00	3.00E-01
				Sc1	2.92E+00	5.37E-02	2.67E-01	7.00E-02	3.91E-01
				Sc3	2.38E-01	5.28E-04	7.59E-02	0.00E+00	7.64E-02
2303-17-5	Tri-allate	4.10E-01	Herbicide	Sc2	8.54E-02	3.70E-04	0.00E+00	0.00E+00	3.70E-04
				Sc1	2.76E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	8.05E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00

The table below gives per substance for Sc3 and updated PNECs information for the site (Fs,site) and country (Fs,country) frequency of exceedances in Fspat, the calculation of Ftemp by all sites (Ftemp_1) and excluding sites with a single measurement that exceeds PNEC (Ftemp_2), the size of the exceedance extent in Fext, the percentage (from the total number of samples) of samples that exceed PNEC and the total amount of samples.

Substance	PNEC (µg/L)	Type	Fs,site	Fs,country	Ftemp_1	Ftemp_2	EXCextent	Exceeding samples (%)	Number of samples (Sc3)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	3.77E-01	7.14E-01	7.13E-01	5.21E-01	9.83E+00	22.91	323
17-beta-Estradiol	4.00E-04	Estrogen	1.22E-01	4.44E-01	7.39E-01	5.58E-01	2.16E+00	6.93	462
2,6-Di-tert-butyl-4-methylphenol	3.16	Antioxidant	4.15E-03	0.00E+00	1.67E-01	1.67E-01	3.16E-01	0.19	1032
2-Ethylhexyl-4-methoxycinnamate	6	Sunscreen	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.00E-01	0.00	543
Acetamiprid	0.5	Neonicotinoid Insecticide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.50E-02	0.00	2221
Azithromycin	0.019	Antibiotic	2.50E-01	5.79E-01	7.69E-01	6.24E-01	8.82E+00	16.07	915
Clarithromycin	0.12	Antibiotic	1.36E-01	2.08E-01	4.07E-01	3.95E-01	2.48E+00	7.74	2792
Clothianidin	0.13	Neonicotinoid Insecticide	5.83E-03	4.17E-02	2.85E-01	2.85E-01	2.50E-01	0.67	2254
Diclofenac	0.05	Analgesic	5.63E-01	7.20E-01	4.75E-01	4.38E-01	8.78E+00	32.40	6698
Erythromycin	2.00E-01	Antibiotic	1.33E-02	0.00E+00	2.68E-01	1.46E-01	4.25E-01	0.44	2520
Estrone	0.0036	Estrogen	7.11E-02	3.00E-01	6.75E-01	4.81E-01	1.31E+00	4.53	552
Imidacloprid	0.0083	Neonicotinoid Insecticide	3.28E-01	6.36E-01	5.65E-01	4.35E-01	7.67E+00	20.33	1845
Methiocarb	2.00E-03	Insecticide/ Herbicide	7.14E-02	2.86E-01	1.00E+00	1.00E+00	1.13E+01	4.70	127
Oxadiazon	0.088	Herbicide	5.93E-03	4.35E-02	5.50E-01	1.00E-01	5.00E-01	0.11	1847
Thiacloprid	0.01	Neonicotinoid Insecticide	8.20E-02	1.30E-01	2.33E-01	1.89E-01	1.75E+00	2.68	2235
Thiamethoxam	0.042	Neonicotinoid Insecticide	1.21E-02	4.35E-02	7.59E-02	7.59E-02	5.66E-01	0.96	3979
Tri-allate	0.41	Herbicide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.44E-01	0.00	2166

The figure shows a comparison of STE scores obtained by WL dataset for all data scenarios and updated PNECs. Two substances didn't fulfilled the representativity criteria in Sc1 and were not shown on the graph.



Annex 6: Information supporting the removing of substances from the WL

Annex 6.1 Application of removal criteria to the WL dataset and PNEC of 2015.

Substance	PNEC (µg/L) (WL report 2015)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference <15%)	Potential candidate for deselection
Diclofenac	1.00E-01	Analgesic	6.45E-01	6.45E-01	25	6697	2.63	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Clarithromycin	1.30E-01	Antibiotic	5.15E-01	5.15E-01	24	2792	1.34	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Azithromycin	9.00E-02	Antibiotic	3.48E-01	3.51E-01	24	1551	0.59	99.8	yes	0.91	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Erythromycin	2.00E-01	Antibiotic	0.00E+00	0.00E+00	24	2520	0.14	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	0.00E+00	1.67E-01	23	1032	0.08	99.7	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	8.99E-01	1.91E+00	14	323	7.35	50.6	no	112.61	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
17-beta-Estradiol	4.00E-04	Estrogen	6.82E-01	1.17E+00	17	461	1.28	72.8	no	70.90	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Estrone	3.60E-03	Estrogen	5.42E-01	7.96E-01	20	552	0.97	91.6	yes	46.98	no	No (dissimilar STE scores)

Substance	PNEC (µg/L) (WL report 2015)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference <15%)	Potential candidate for deselection
Oxadiazon	8.80E-02	Herbicide	1.00E-01	1.01E-01	23	1847	0.45	99.9	yes	0.72	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Tri-allate	6.70E-01	Herbicide	0.00E+00	3.70E-04	23	2166	0.05	99.9	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Methiocarb	1.00E-02	Insecticide / Herbicide	4.45E-01	9.08E-01	22	1798	1.00	98.0	yes	103.84	no	No (dissimilar STE scores)
Imidacloprid	9.00E-03	Neonicotinoid Insecticide	7.31E-01	1.01E+00	22	1830	3.67	72.5	no	37.76	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Clothianidin	1.30E-01	Neonicotinoid Insecticide	2.86E-01	2.86E-01	24	2254	0.25	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Thiamethoxam	1.40E-01	Neonicotinoid Insecticide	6.15E-02	6.15E-02	24	4020	0.09	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Acetamiprid	5.00E-01	Neonicotinoid Insecticide	0.00E+00	0.00E+00	24	2221	0.02	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Thiacloprid	5.00E-02	Neonicotinoid Insecticide	0.00E+00	0.00E+00	24	2243	0.20	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	0.00E+00	6.22E-04	23	543	0.50	99.3	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)

Annex 6.2 Application of removal criteria to the combined dataset and updated PNECs

The short-list of substances, identified as potential candidates to be removed from the WL using WL dataset and the updated PNECs, is confirmed applying the removal criteria to the combined dataset together with updated PNECs except for thiacloprid. For all other substances the STE scores found by both datasets are identical which confirms the similarity of the assessment of these substances.

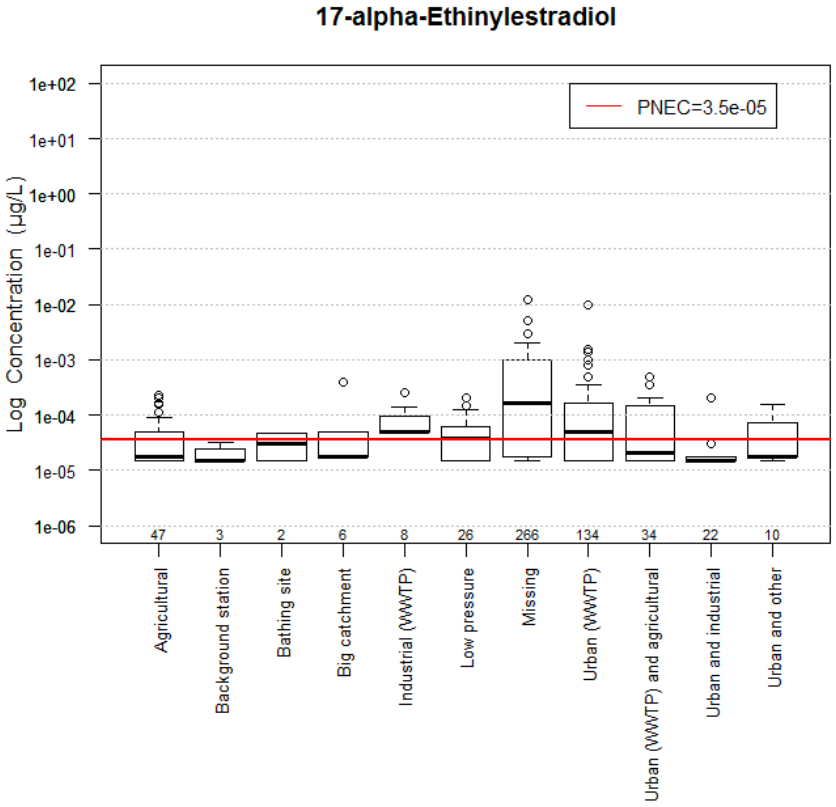
Substance	PNEC (µg/L)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference<15%)	Potential candidate for deselection
Diclofenac	5.00E-02	Analgesic	1.215	1.215	26	17748	9.21	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Clarithromycin	1.20E-01	Antibiotic	0.406	0.406	25	7443	1.08	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Azithromycin	1.90E-02	Antibiotic	1.219	1.537	20	1217	8.95	44.8	no	26.06	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Erythromycin	2.00E-01	Antibiotic	0.000	0.000	25	6313	0.25	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	0.000	0.080	23	1293	0.08	99.8	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	0.862	1.704	14	469	5.85	58.7	no	97.78	no	No (no LOQ-PNEC criterion; dissimilar STE scores)

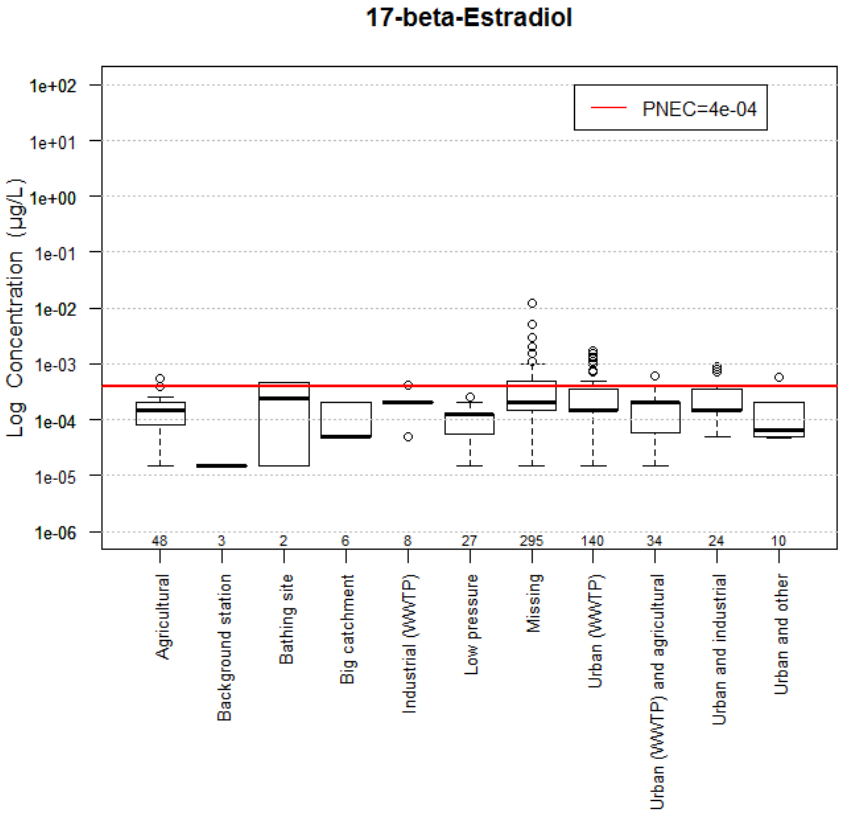
Substance	PNEC (µg/L)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference<15%)	Potential candidate for deselection
17-beta-Estradiol	4.00E-04	Estrogen	0.829	1.403	20	716	2.50	35.4	no	69.13	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Estrone	3.60E-03	Estrogen	0.521	0.645	23	1314	1.39	95.5	yes	23.85	no	No (dissimilar STE scores)
Oxadiazon	8.80E-02	Herbicide	0.277	0.268	23	50148	0.28	99.6	yes	3.13	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Tri-allate	4.10E-01	Herbicide	0.000	0.000	23	20725	0.06	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Methiocarb	2.00E-03	Insecticide/ Herbicide	1.227	2.094	10	2781	7.00	10.0	no	70.71	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Imidacloprid	8.30E-03	Neonicotinoid Insecticide	1.299	1.729	22	24745	27.71	27.6	no	33.15	no	No (no LOQ-PNEC criterion; dissimilar STE scores)
Clothianidin	1.30E-01	Neonicotinoid Insecticide	0.188	0.188	24	5952	0.19	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Thiamethoxam	4.20E-02	Neonicotinoid Insecticide	0.376	0.436	24	9041	0.36	99.5	yes	15.75	no	No (dissimilar STE scores)
Acetamiprid	5.00E-01	Neonicotinoid Insecticide	0.000	0.000	24	7121	0.02	100.0	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)
Thiacloprid	1.00E-02	Neonicotinoid Insecticide	0.237	0.403	23	8533	1.00	98.9	yes	70.27	no	No (dissimilar STE scores)

Substance	PNEC (µg/L)	Type	STE (Sc3)	STE (Sc2)	Number of countries (Sc3)	Number of samples (Sc3)	RQ (P95) for Sc3	Non-quantified samples with 0.5*LOQ≤PNEC in Sc2 (% from total)	LOQ-PNEC criterion for Sc2 (>90%)	Difference of STE scores (%)	Similar STE scores (difference<15%)	Potential candidate for deselection
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	0.000	0.001	23	543	0.50	99.3	yes	0.00	yes	Yes (fulfils LOQ-PNEC criterion; similar STE scores)

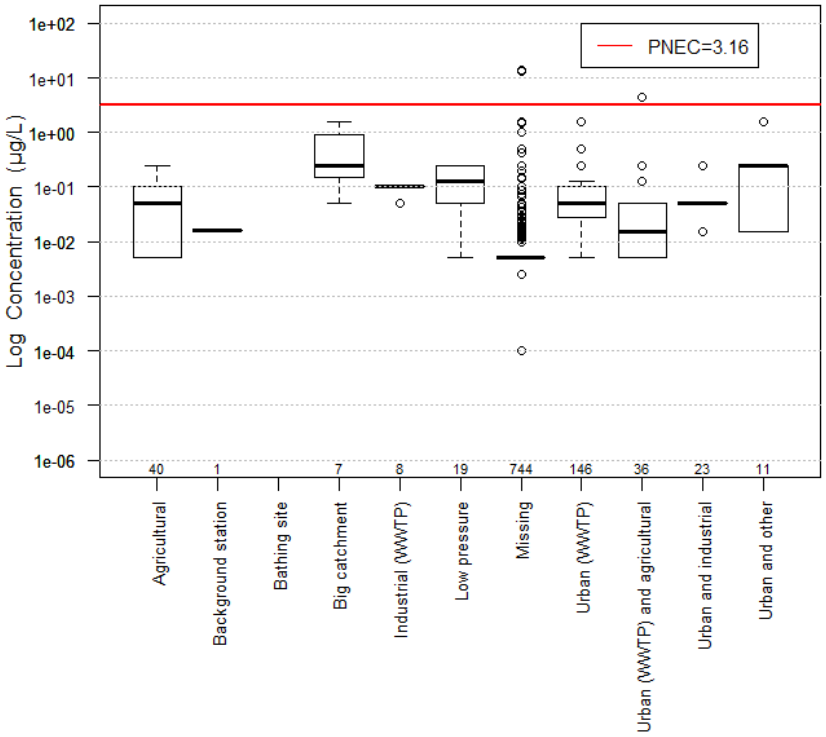
Annex 7: Additional information for WL substances

Annex 7.1 WL dataset in Sc2 and updated PNECs: Nearby pressures

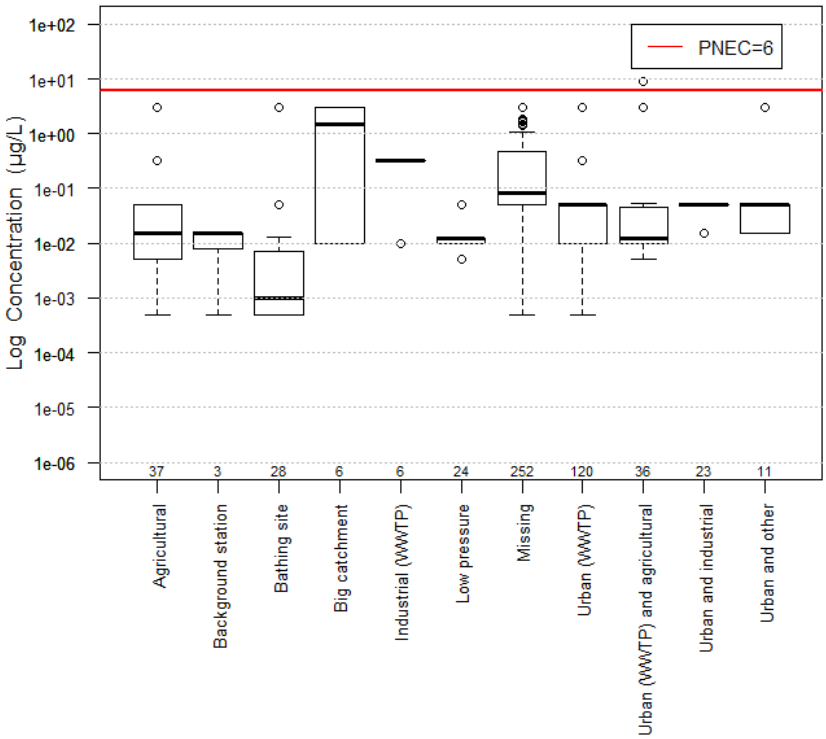




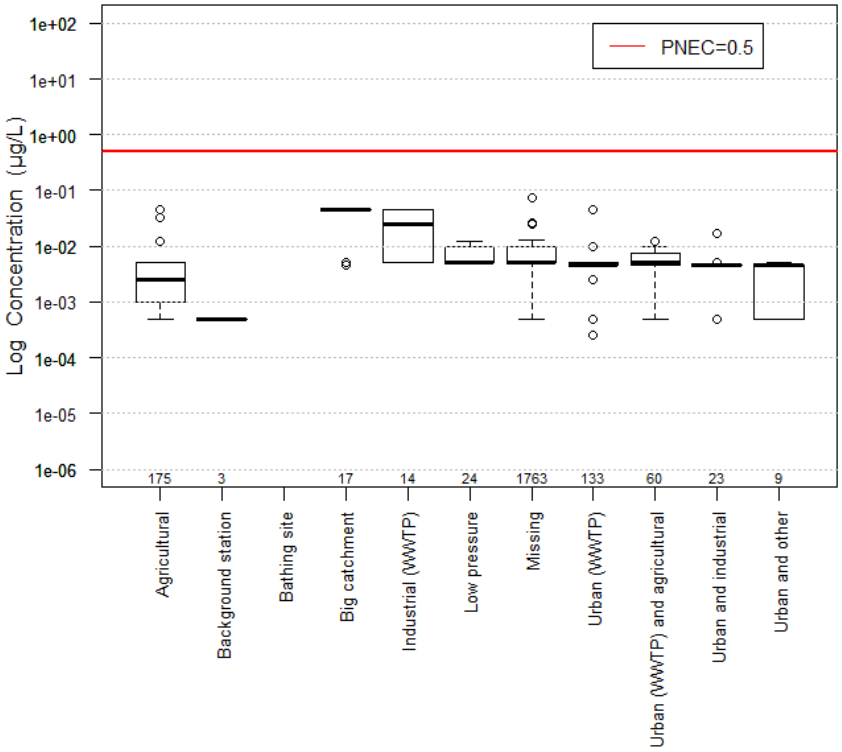
2,6-Di-tert-butyl-4-methylphenol



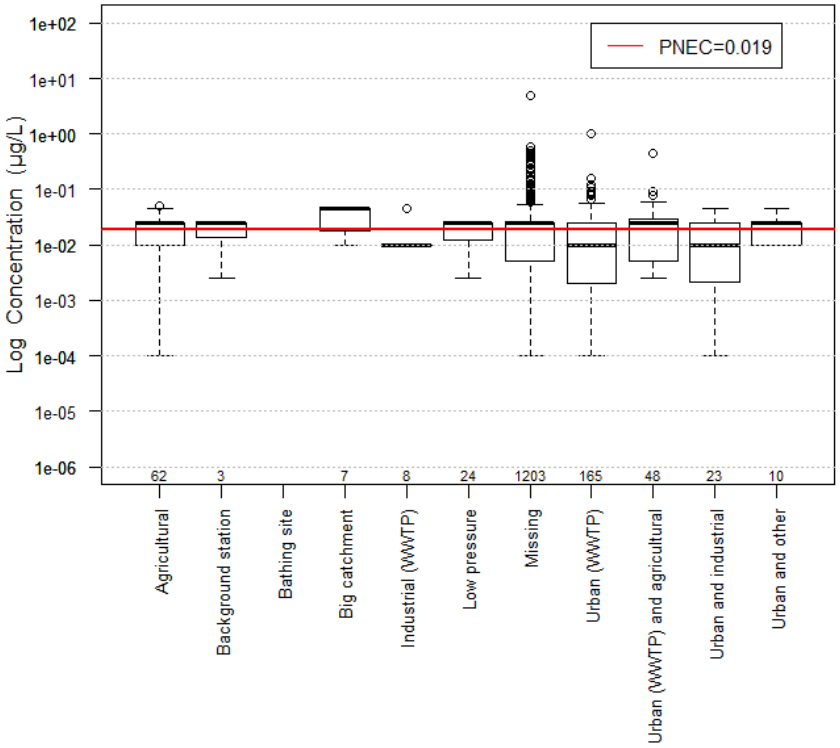
2-Ethylhexyl-4-methoxycinnamate



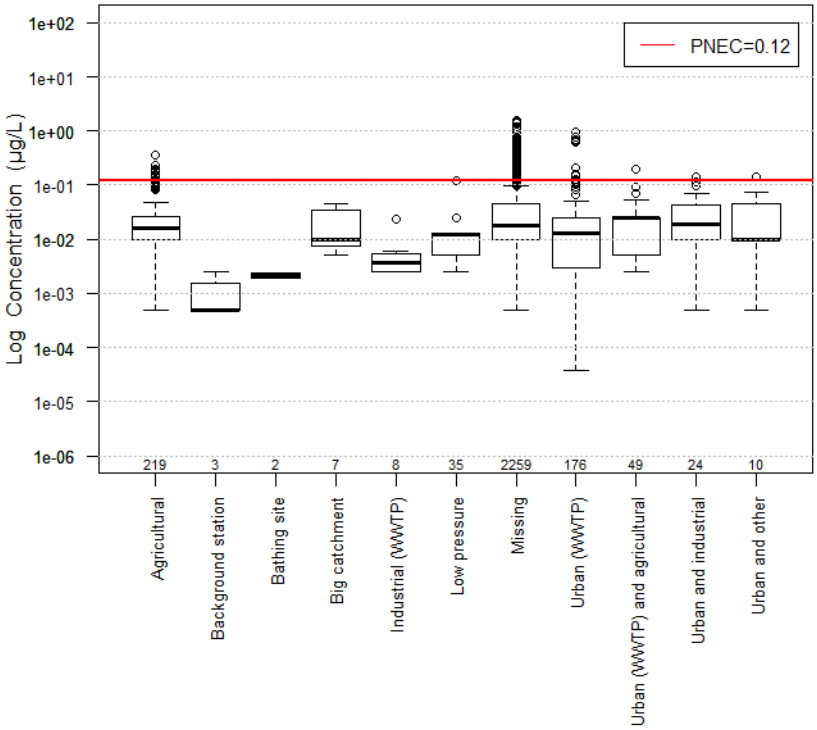
Acetamiprid



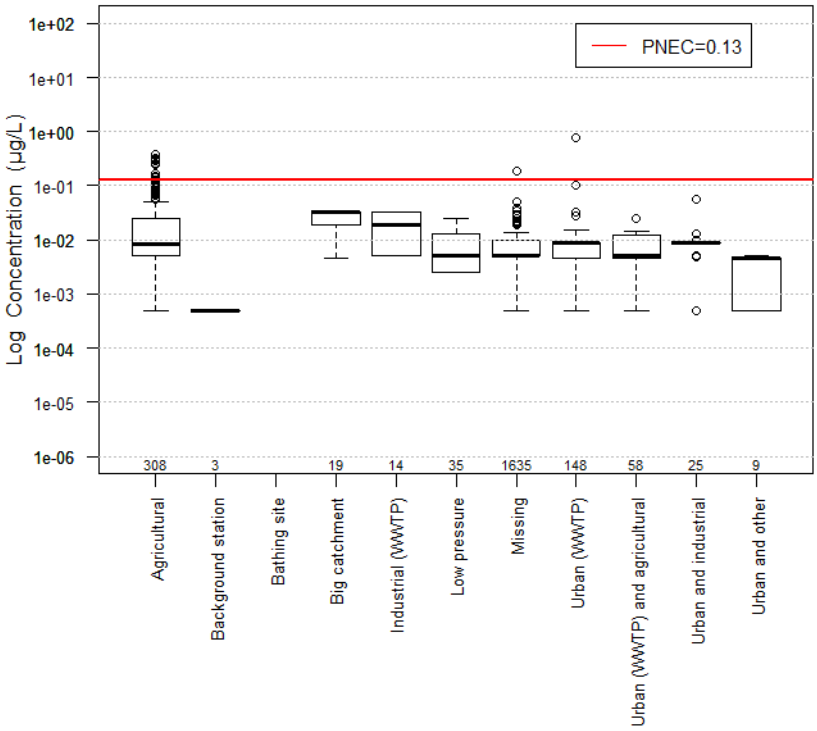
Azithromycin



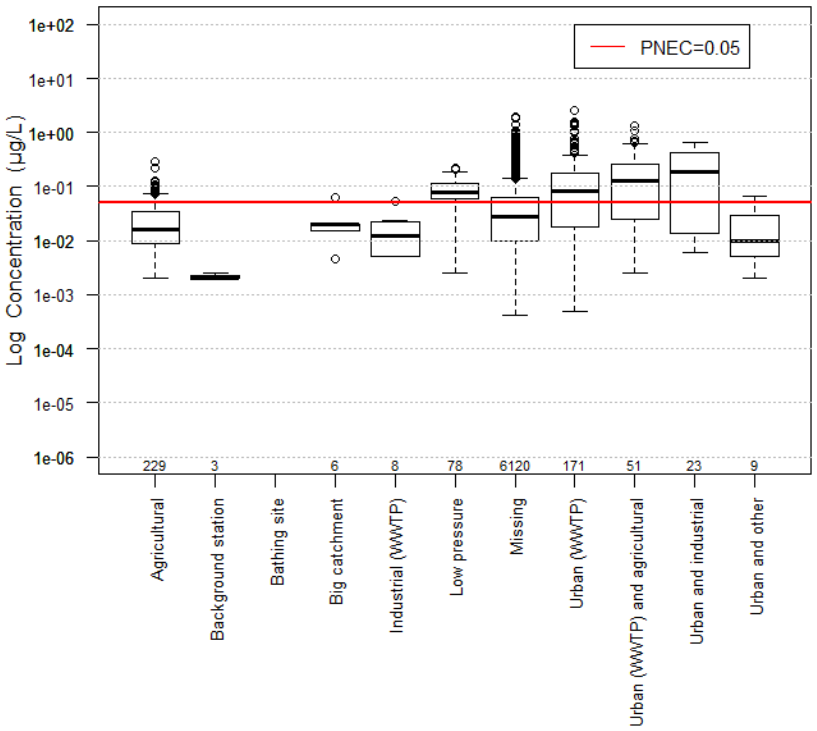
Clarithromycin



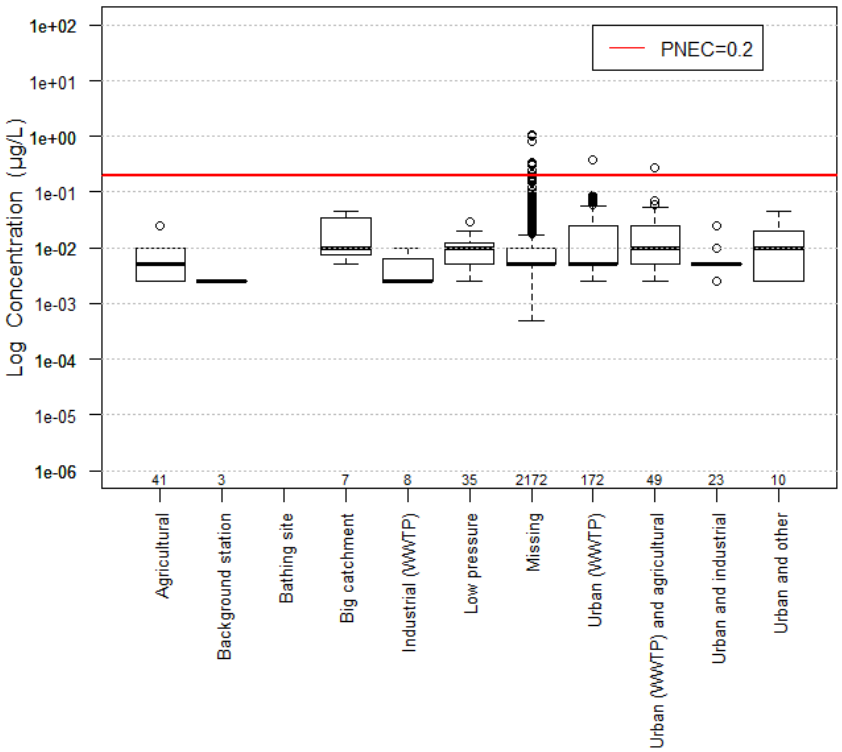
Clothianidin



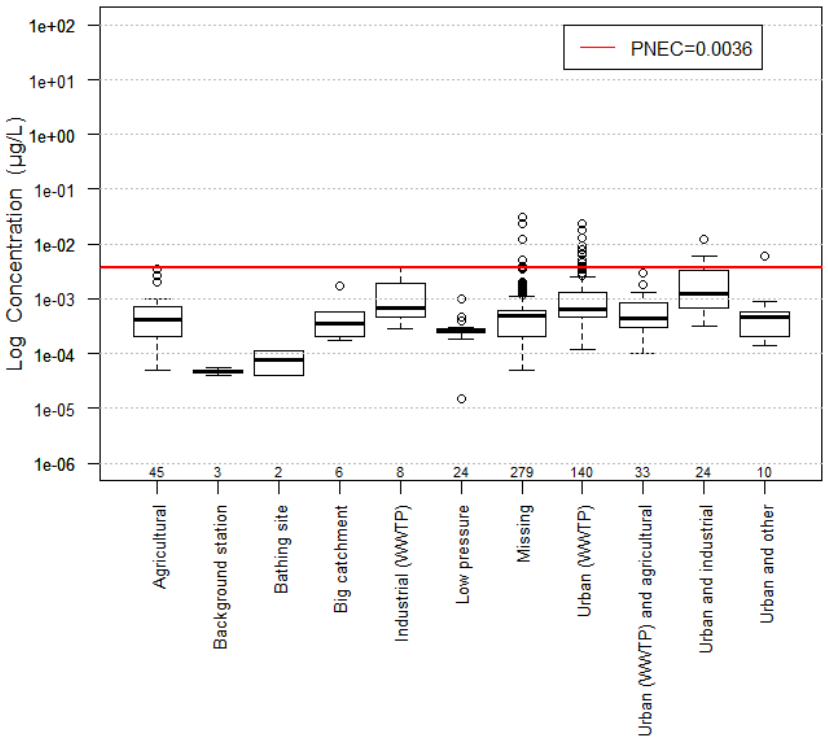
Diclofenac



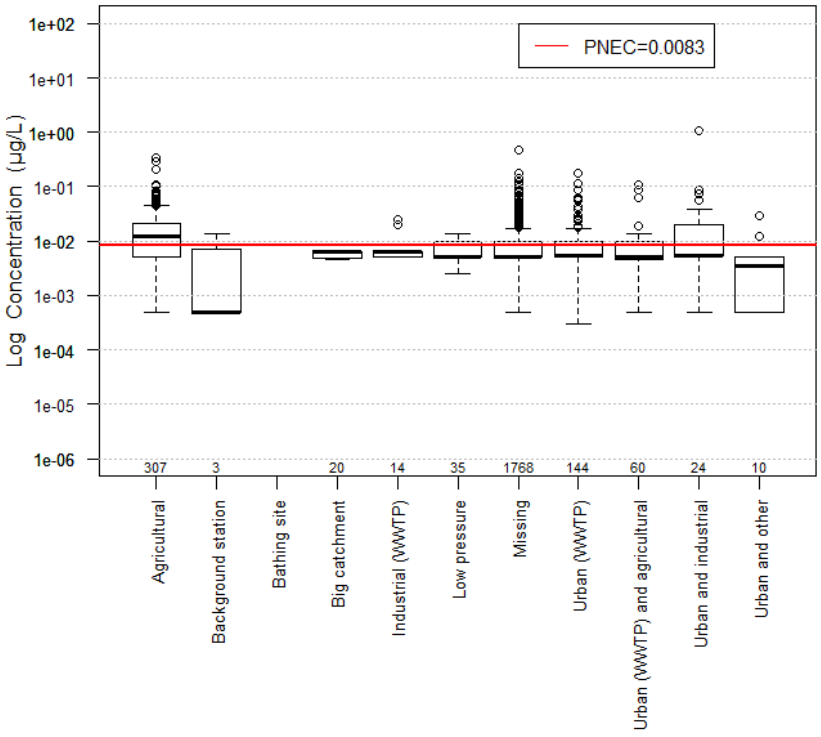
Erythromycin



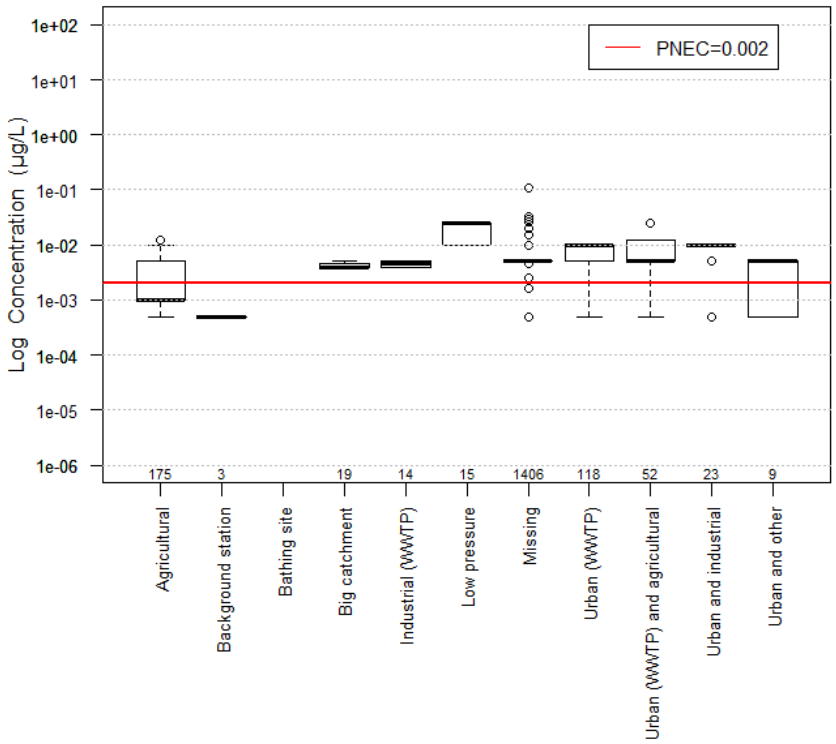
Estrone



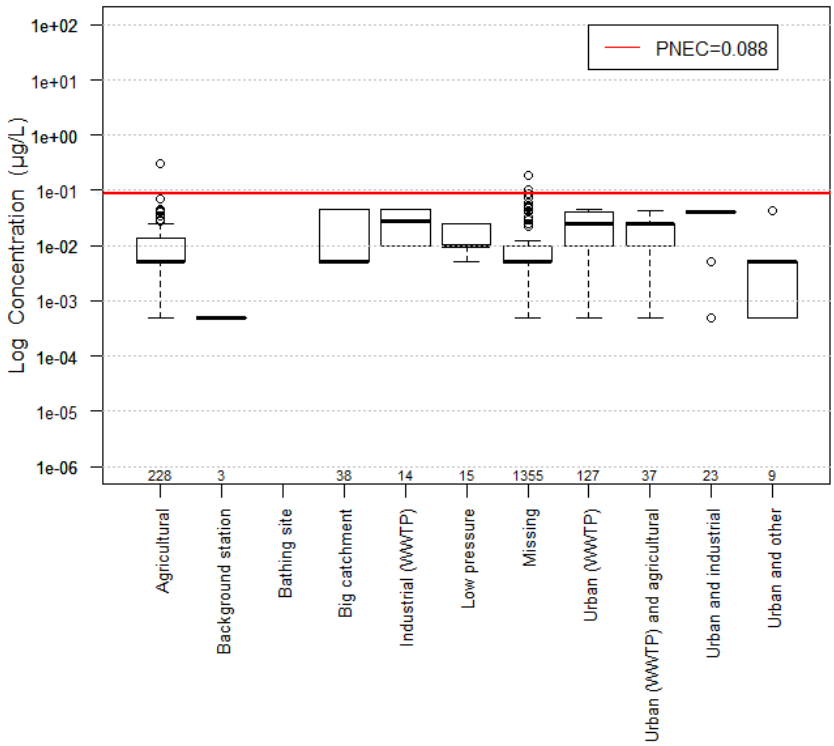
Imidacloprid



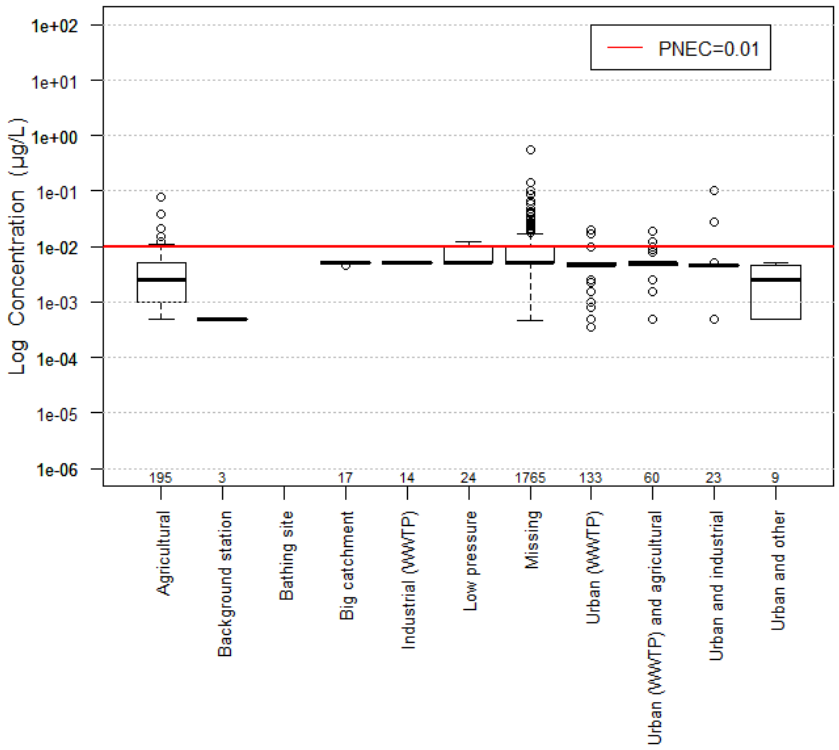
Methiocarb



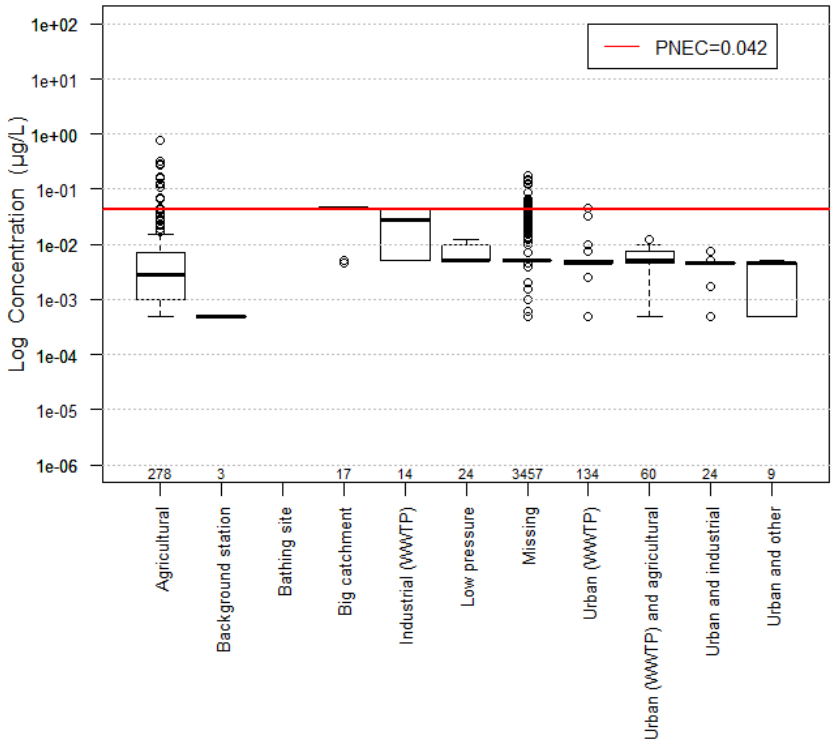
Oxadiazon

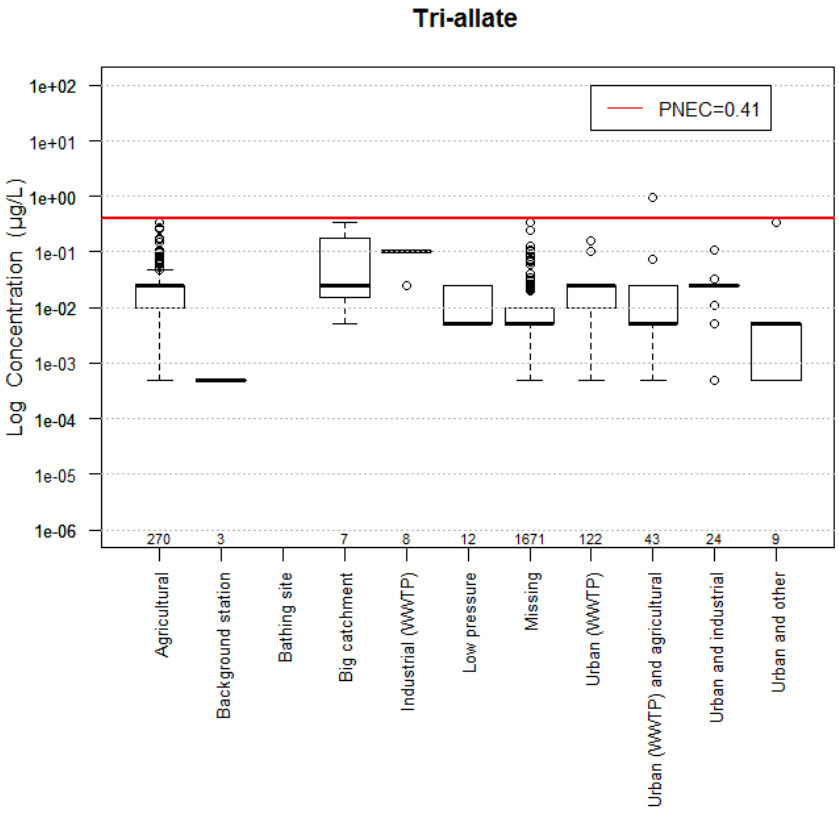


Thiacloprid



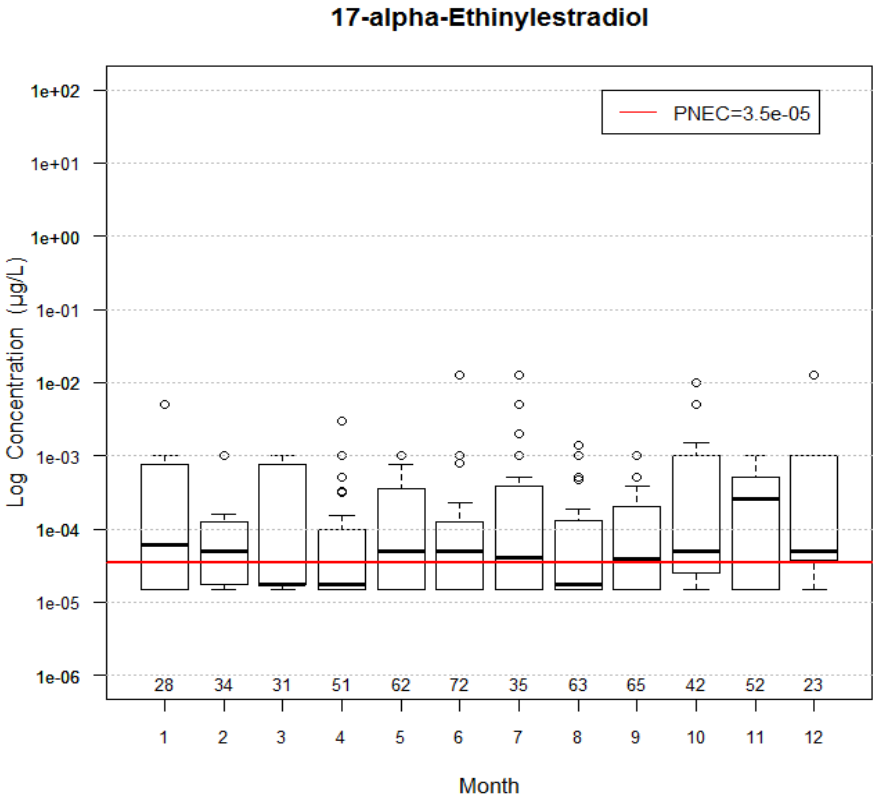
Thiamethoxam

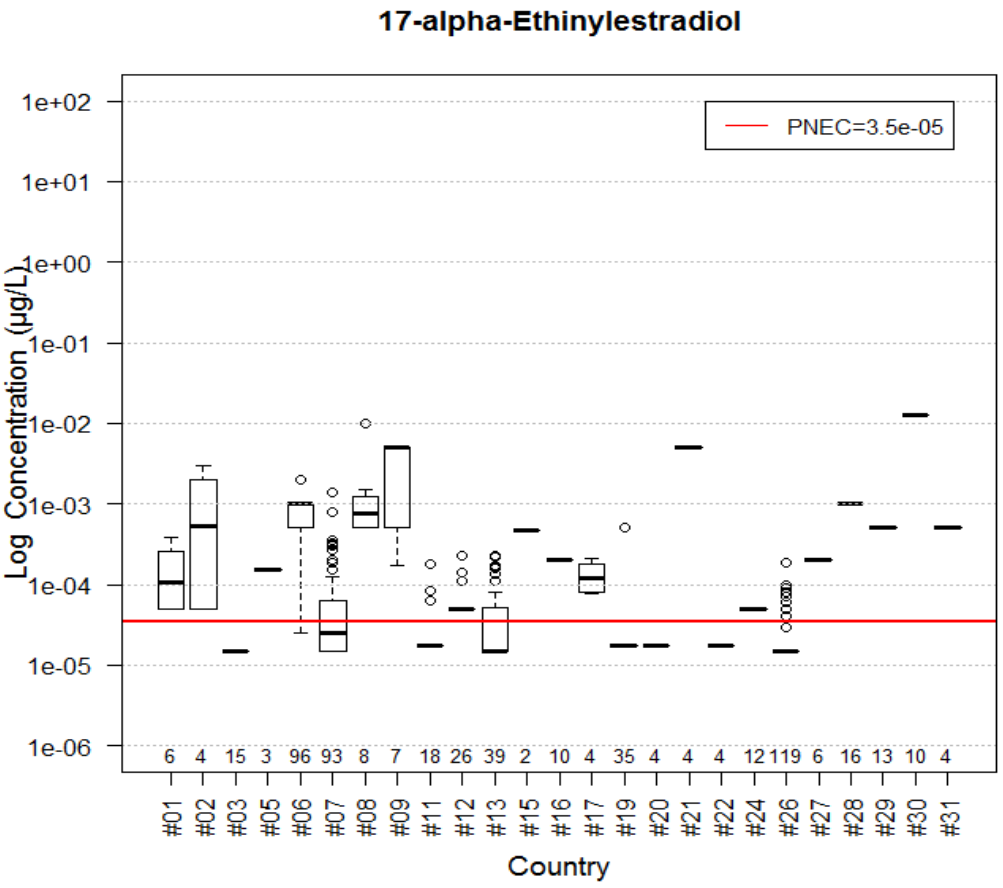



Tri-allate
PNEC=0.41
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
270
3
7
8
12
1671
122
43
24
9
Agricultural
Background station
Bathing site
Big catchment
Industrial (WWTP)
Low pressure
Missing
Urban (WWTP)
Urban (WWTP) and agricultural
Urban and industrial
Urban and other

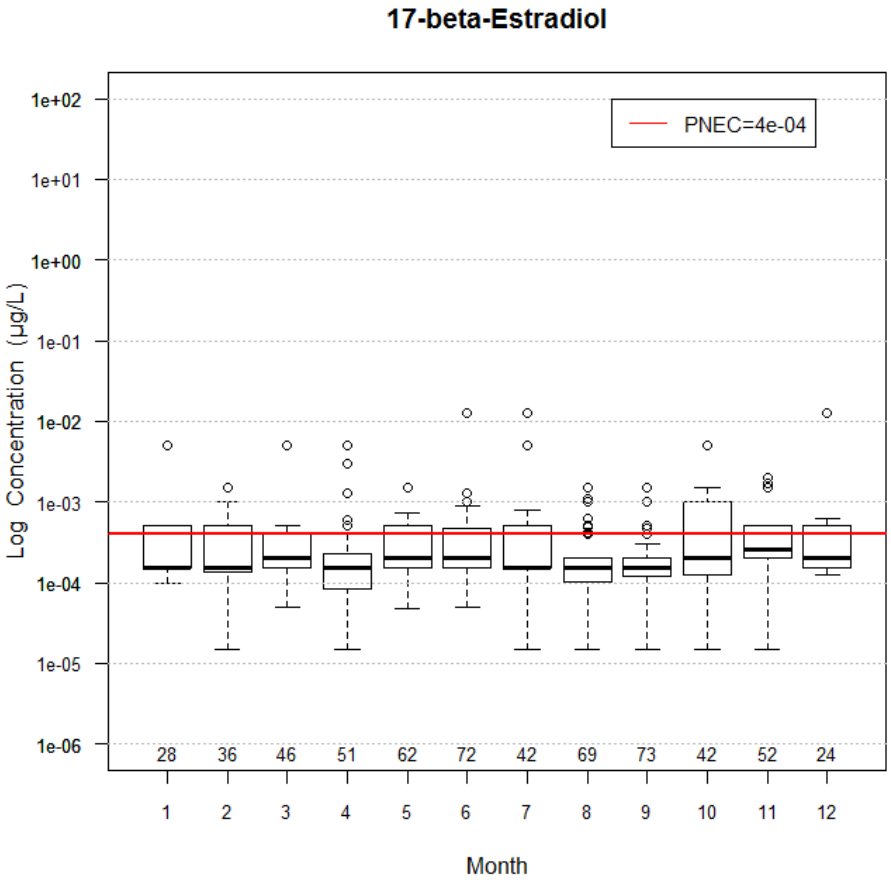
Annex 7.2 WL dataset in Sc2 and updated PNECs: Seasonality and Concentrations per country

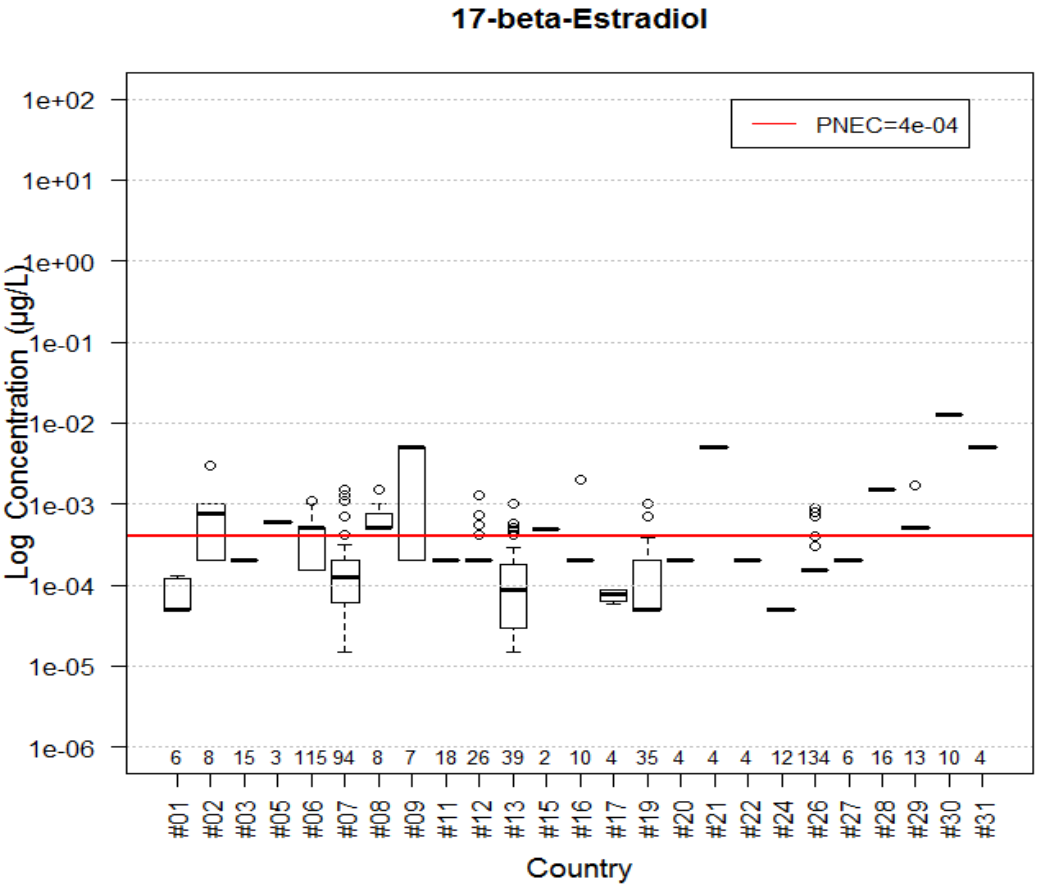
17-alpha-Ethinylestradiol



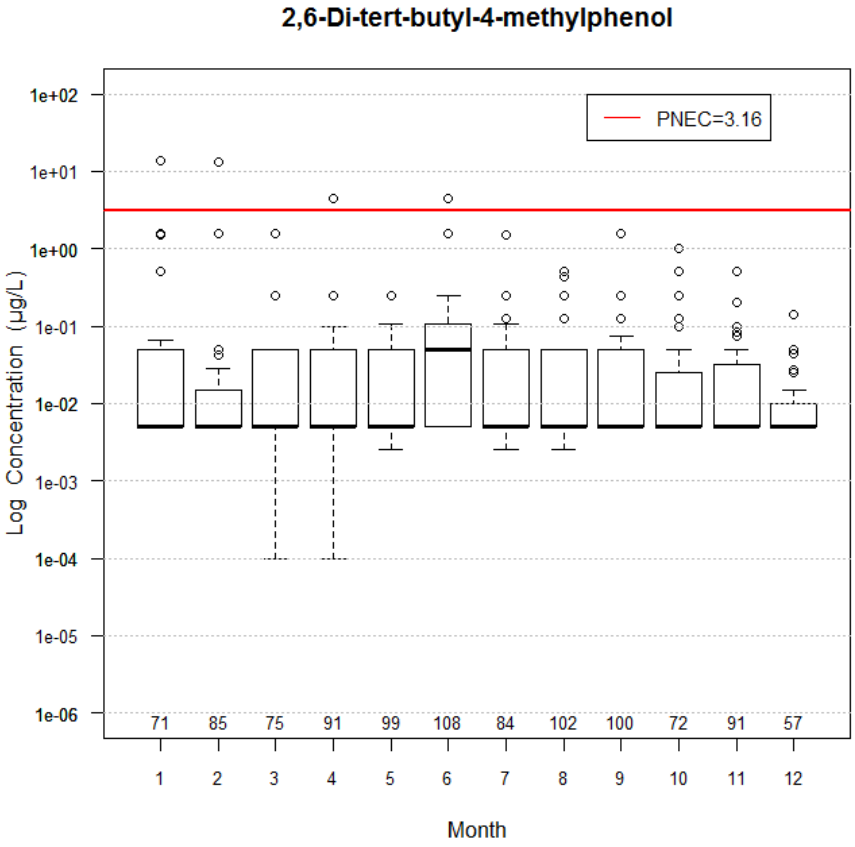


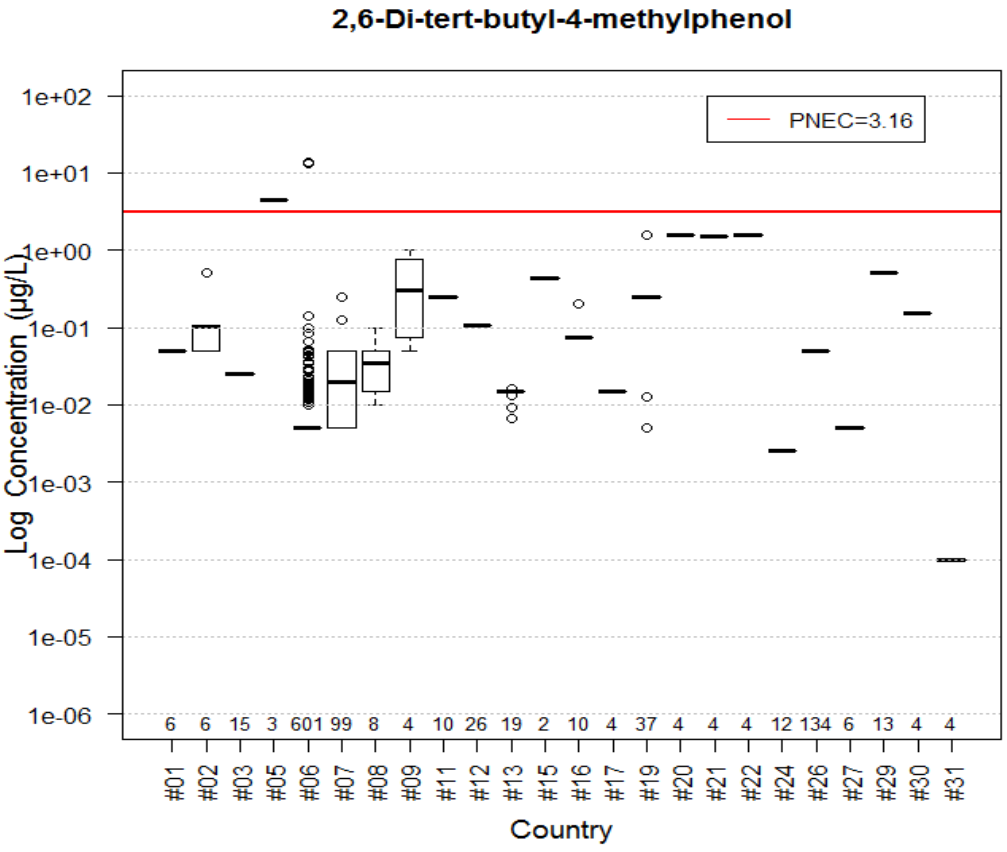
17-beta-Estradiol



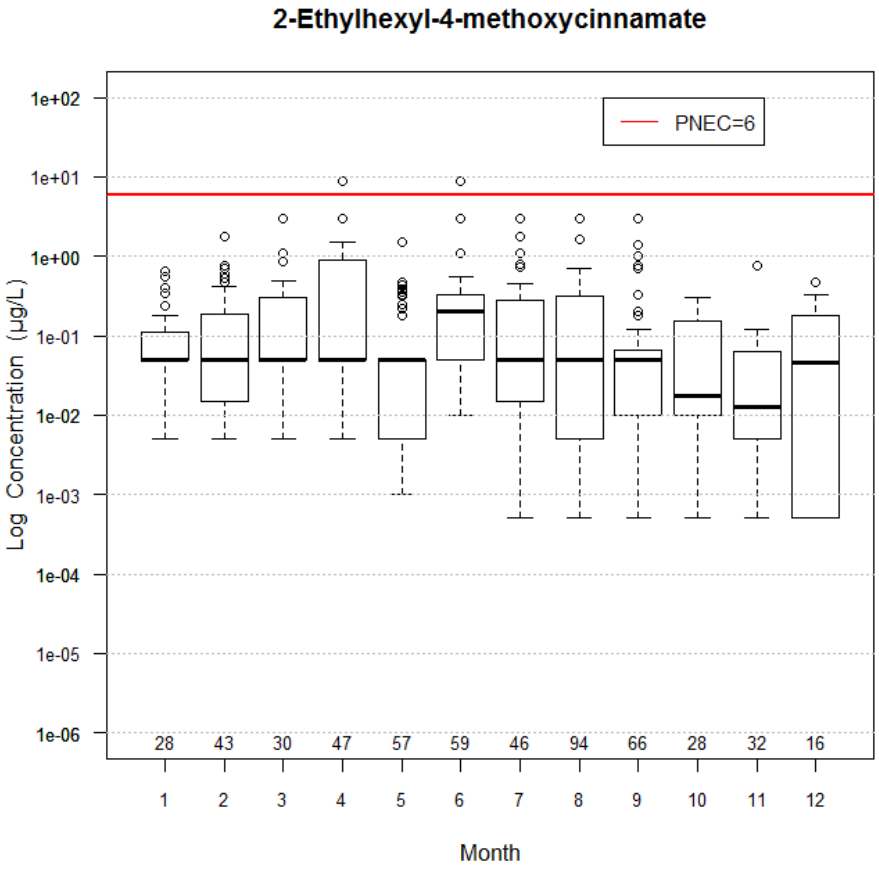


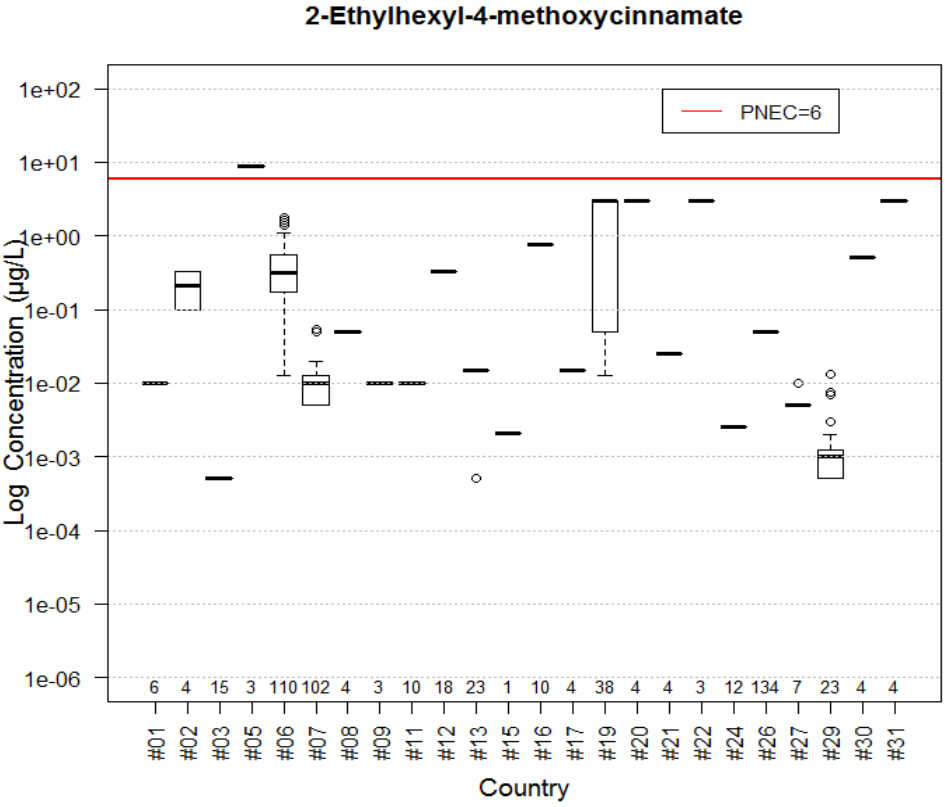
2,6-Di-tert-butyl-4-methylphenol



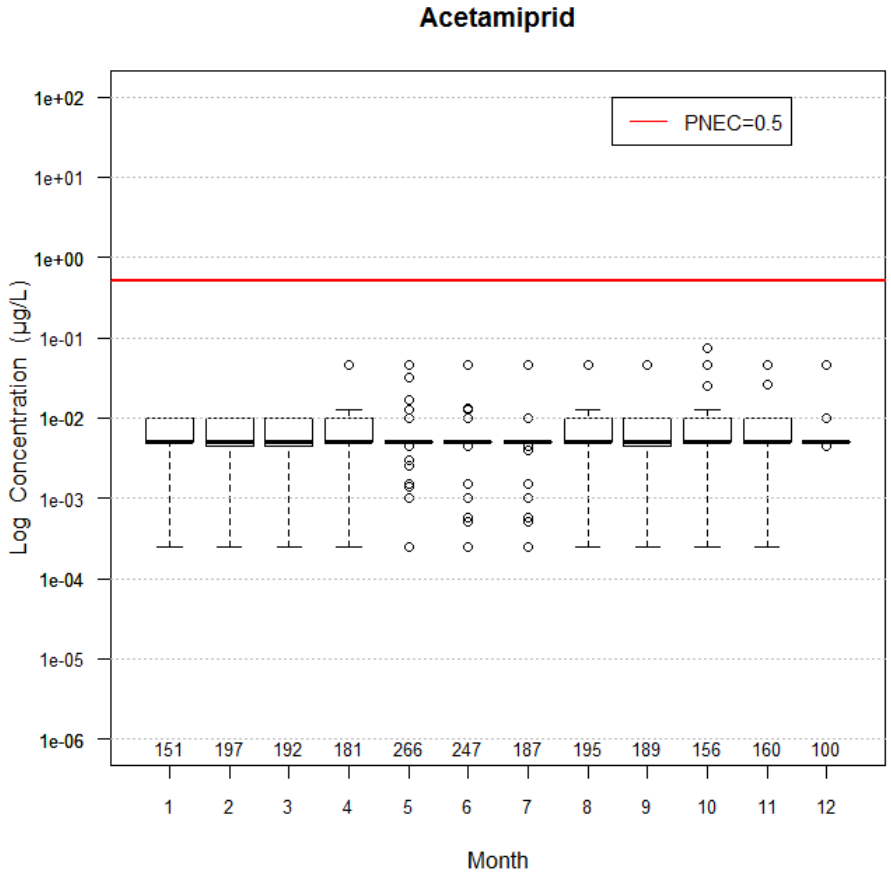


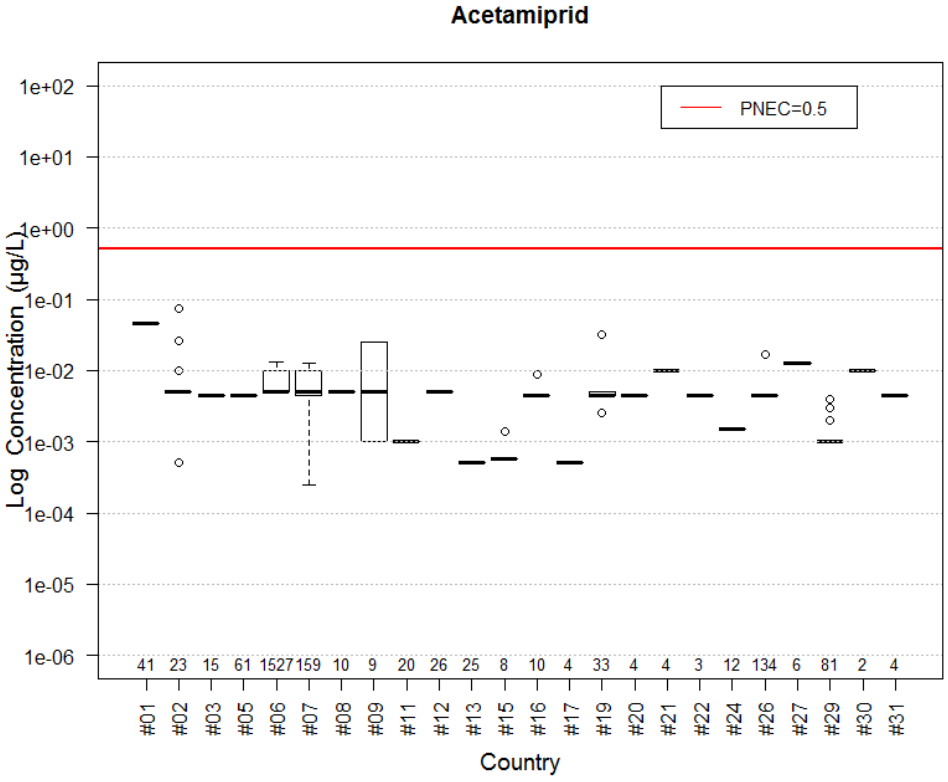
2-Ethylhexyl-4-methoxycinnamate



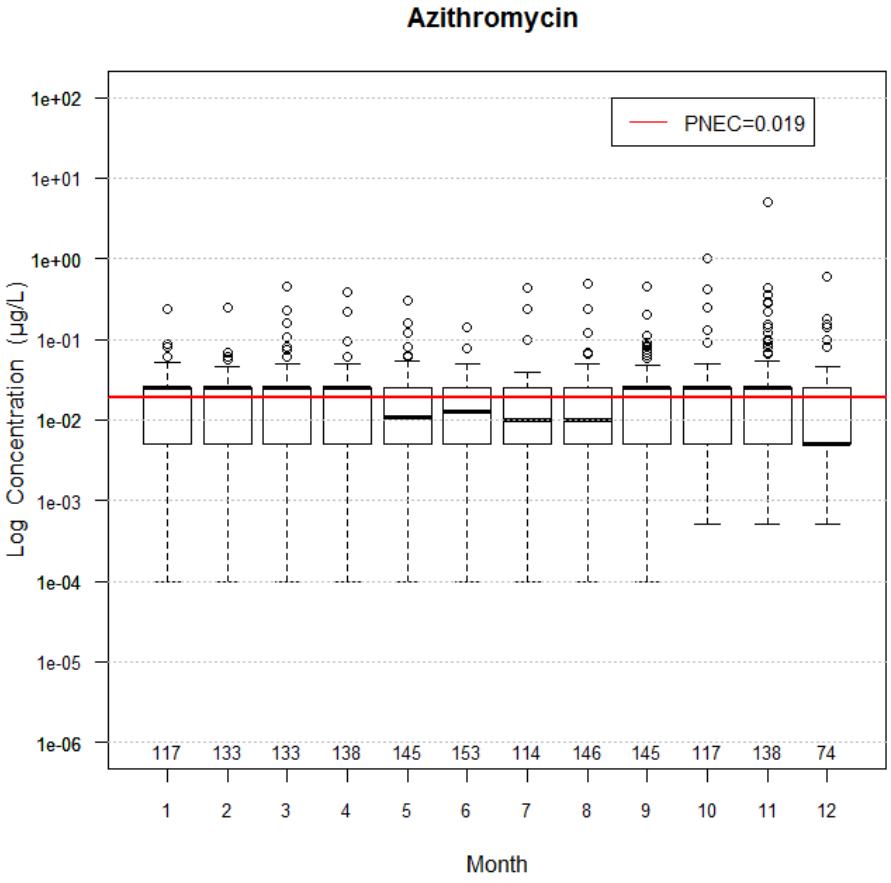


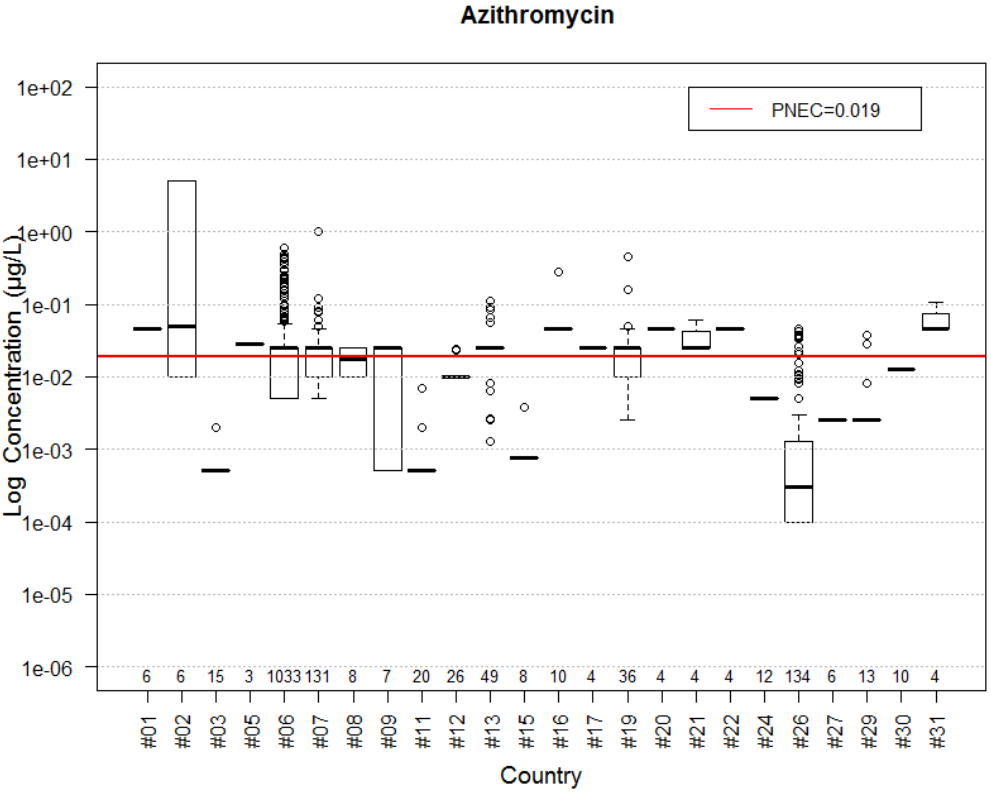
Acetamiprid



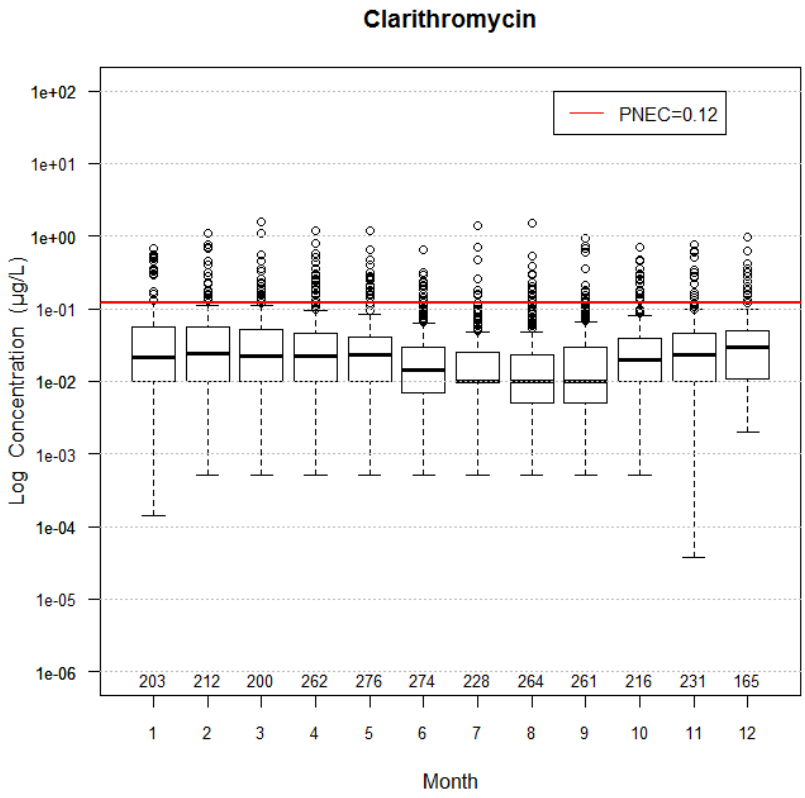


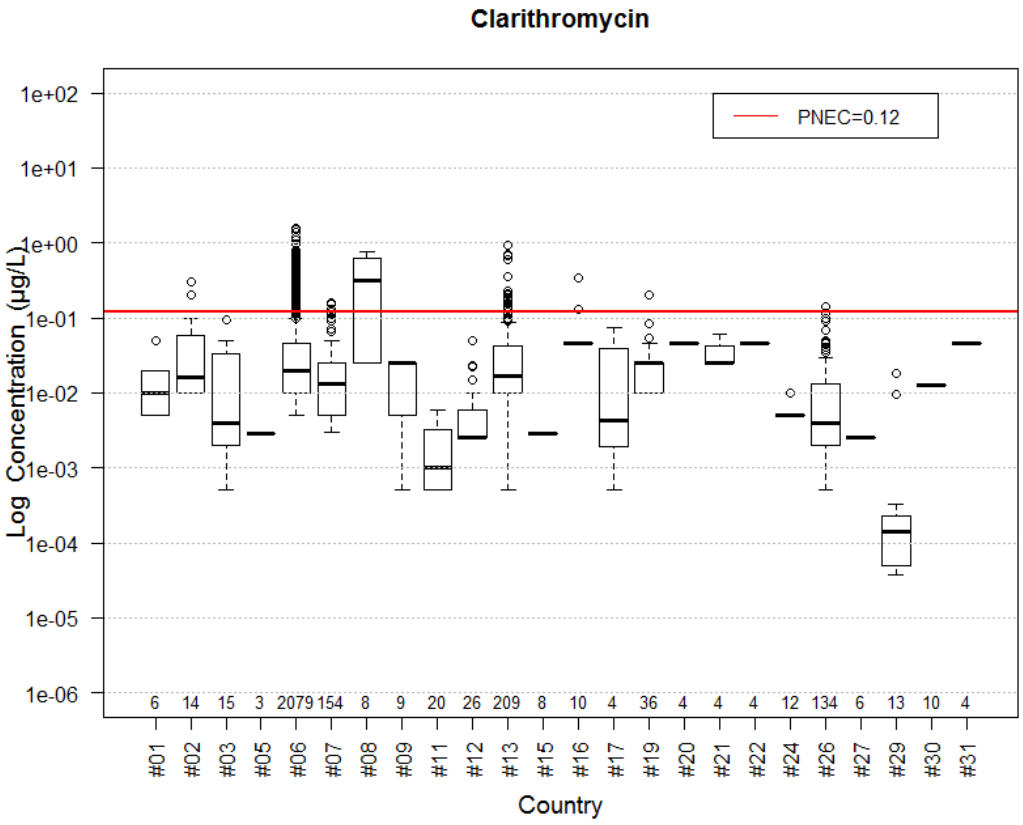
Azithromycin



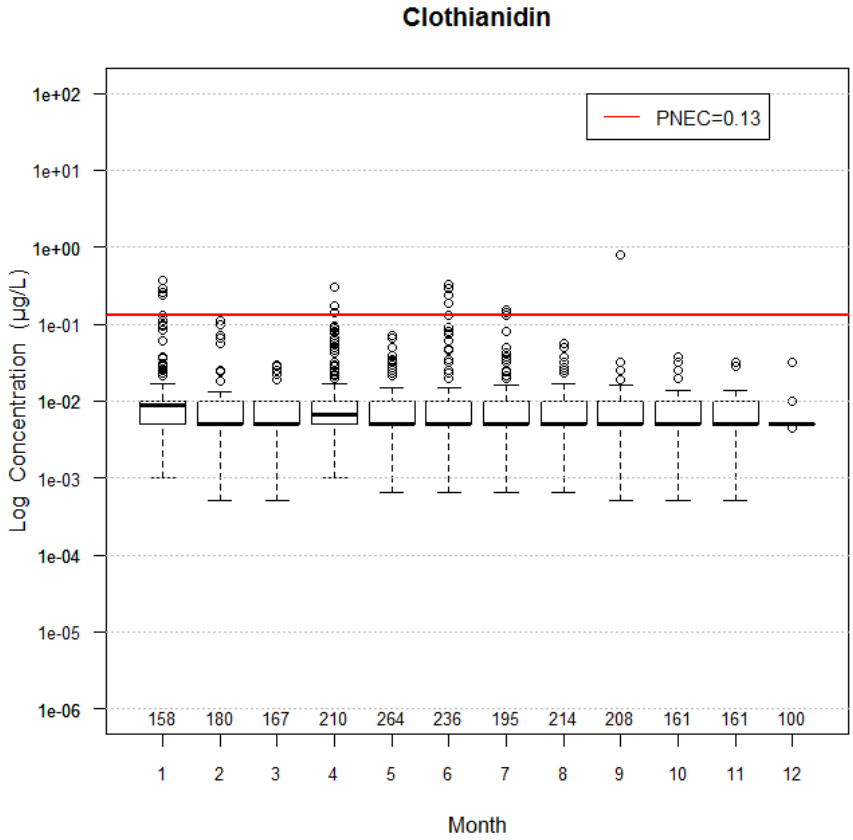


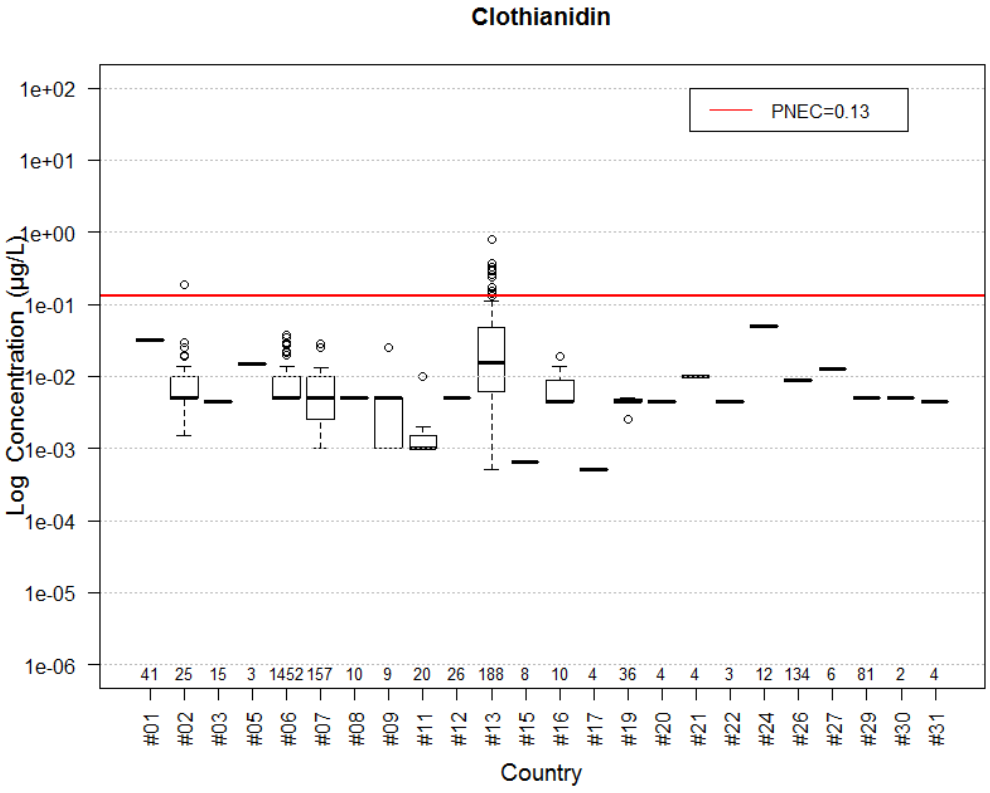
Clarithromycin



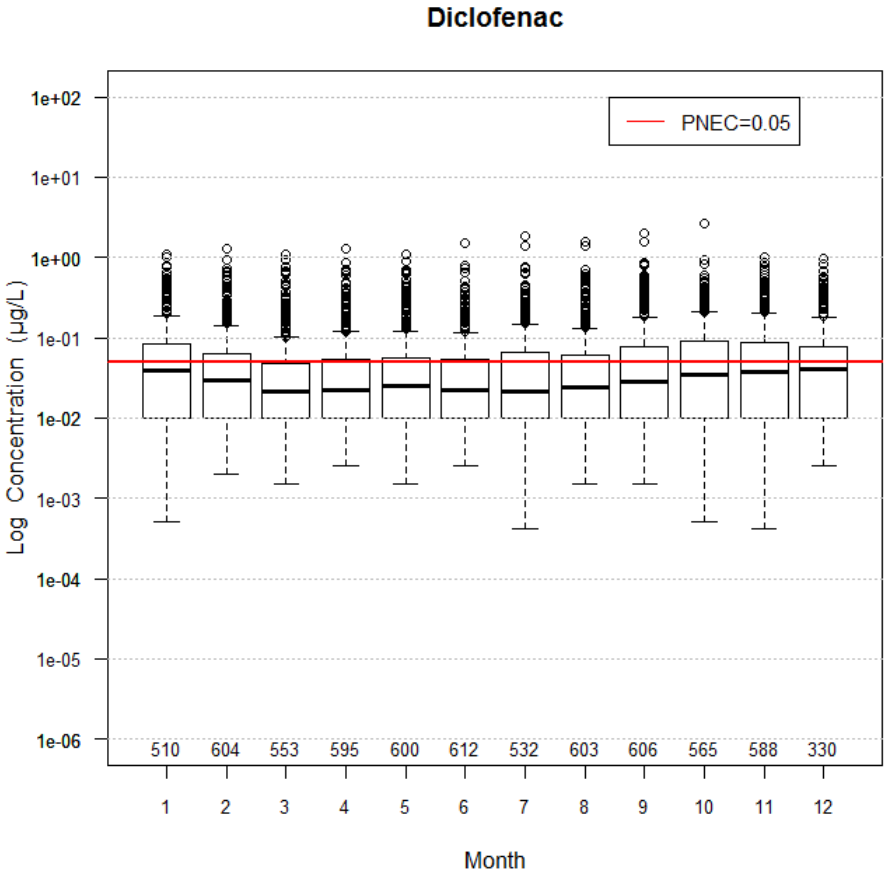


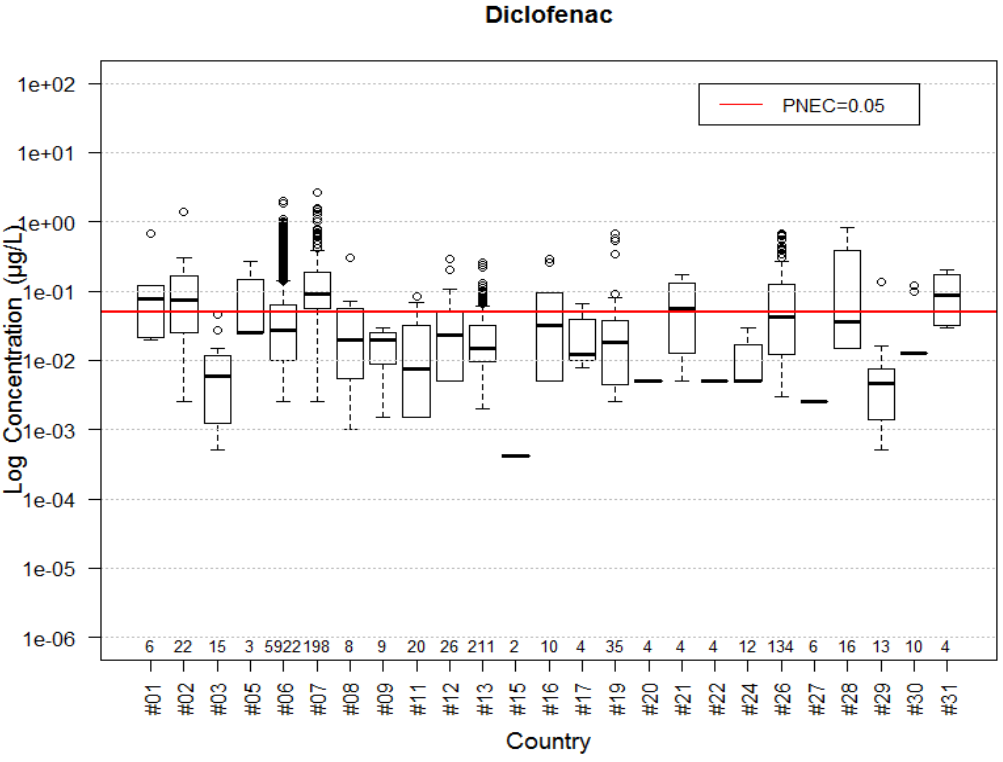
Clothianidin



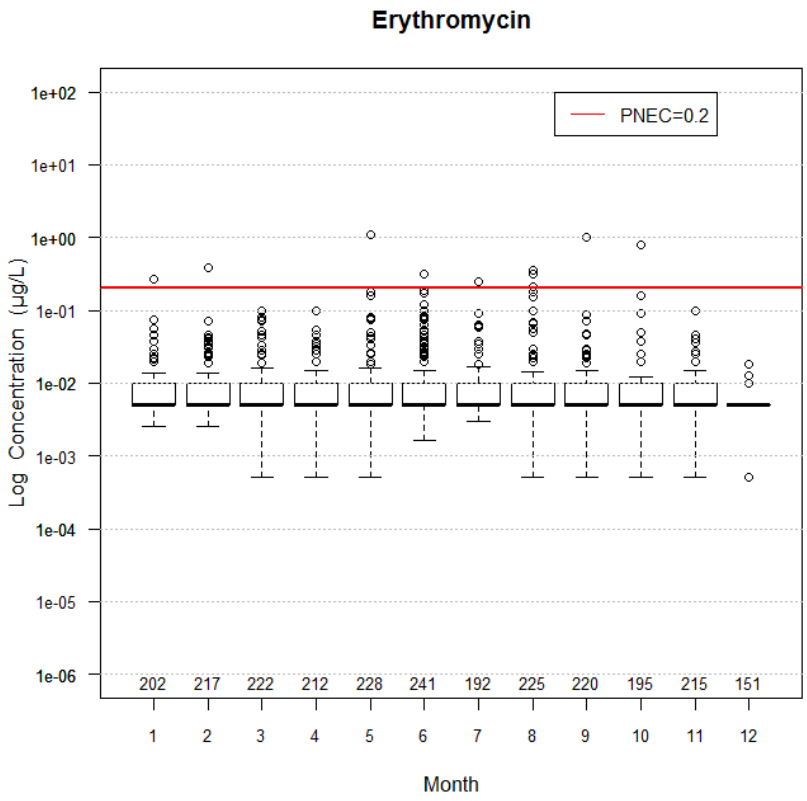


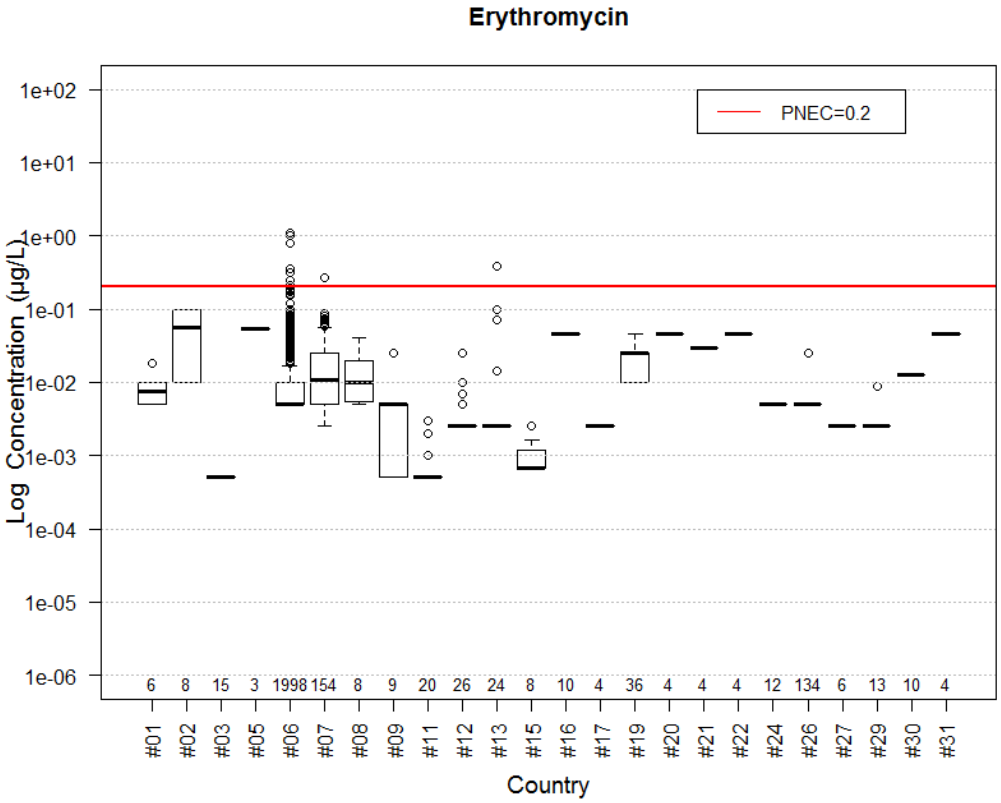
Diclofenac


Diclofenac
PNEC=0.05
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
510 604 553 595 600 612 532 603 606 565 588 330
1 2 3 4 5 6 7 8 9 10 11 12
Month

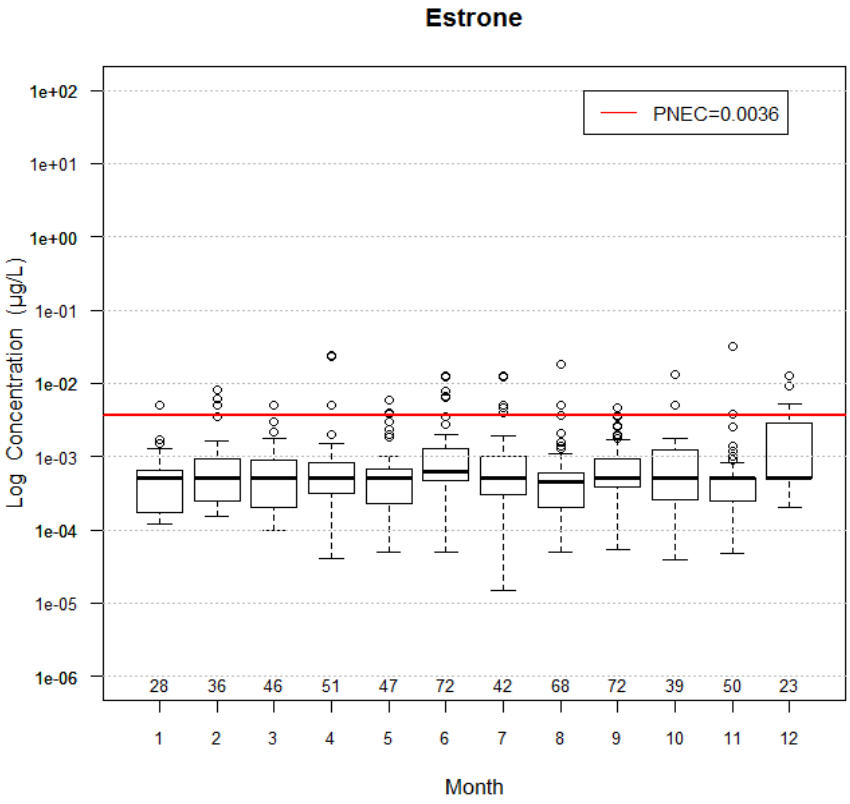

Diclofenac
PNEC=0.05
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
6 22 15 3 592 2198 8 9 20 26 211 2 10 4 35 4 4 4 12 134 6 16 13 10 4
#01 #02 #03 #05 #06 #07 #08 #09 #11 #12 #13 #15 #16 #17 #19 #20 #21 #22 #24 #26 #27 #28 #29 #30 #31
Country

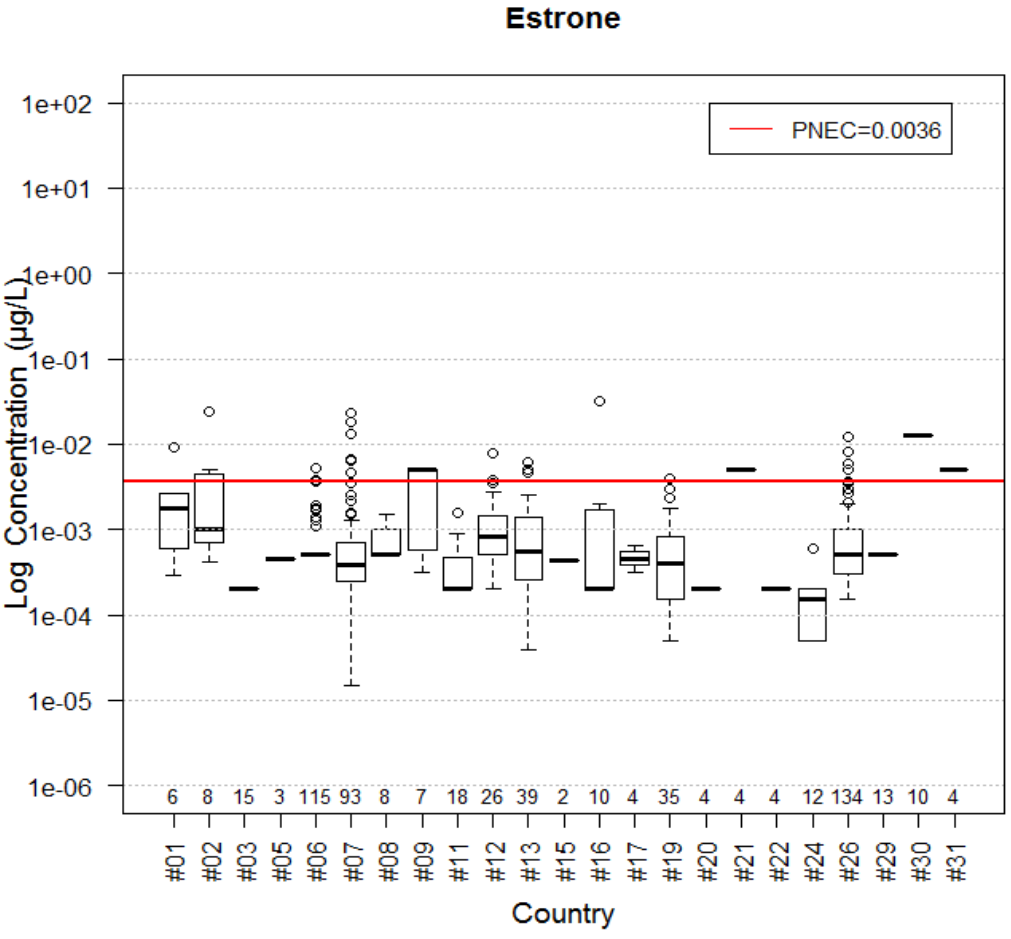
Erythromycin



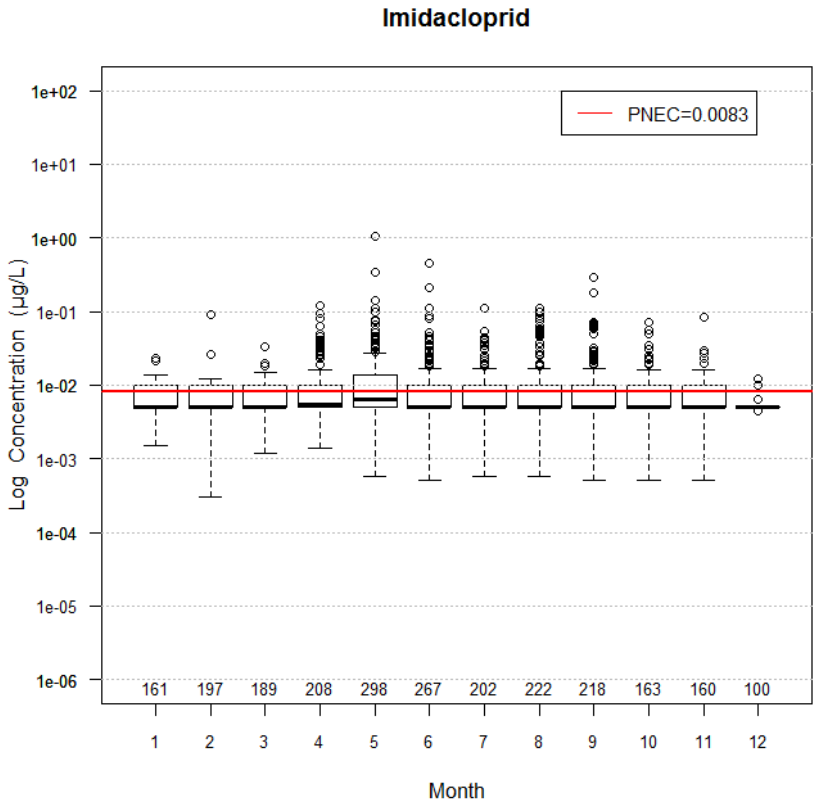


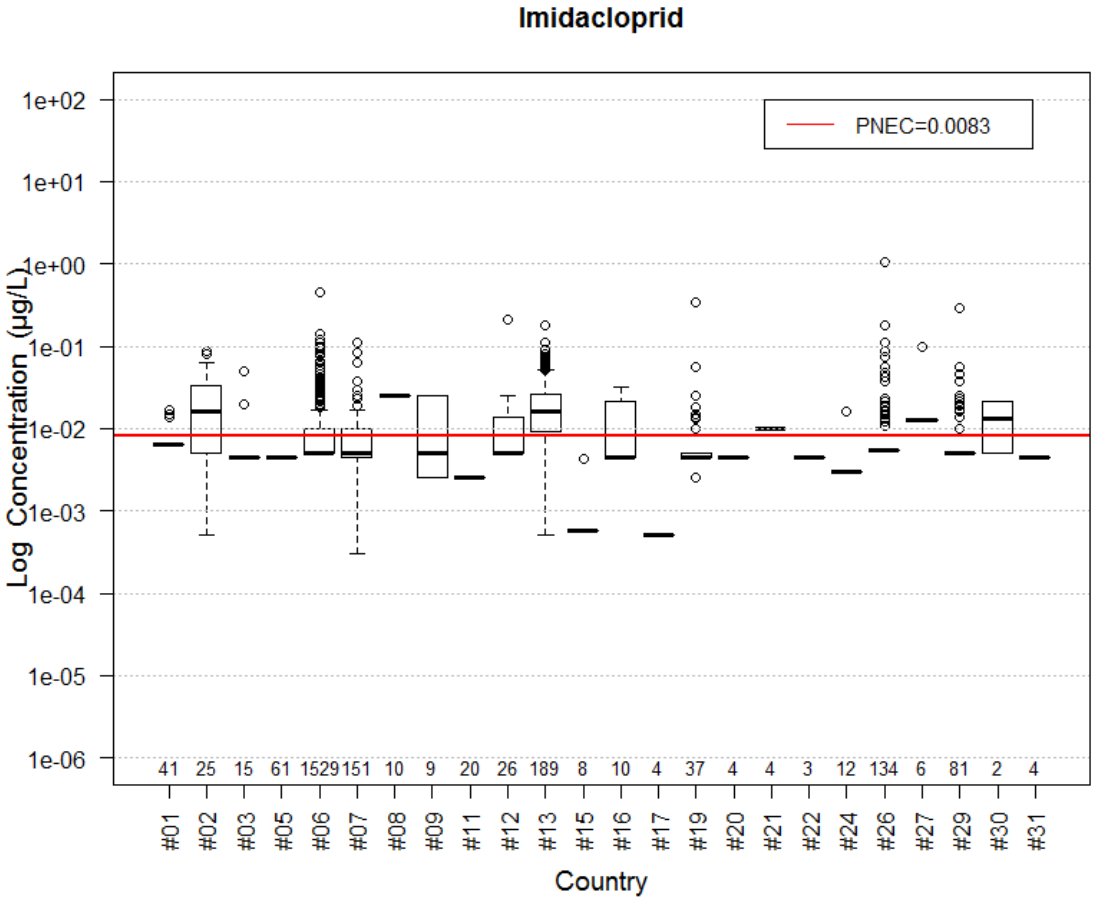
Estrone


Estrone
PNEC=0.0036
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
28 36 46 51 47 72 42 68 72 39 50 23
1 2 3 4 5 6 7 8 9 10 11 12
Month

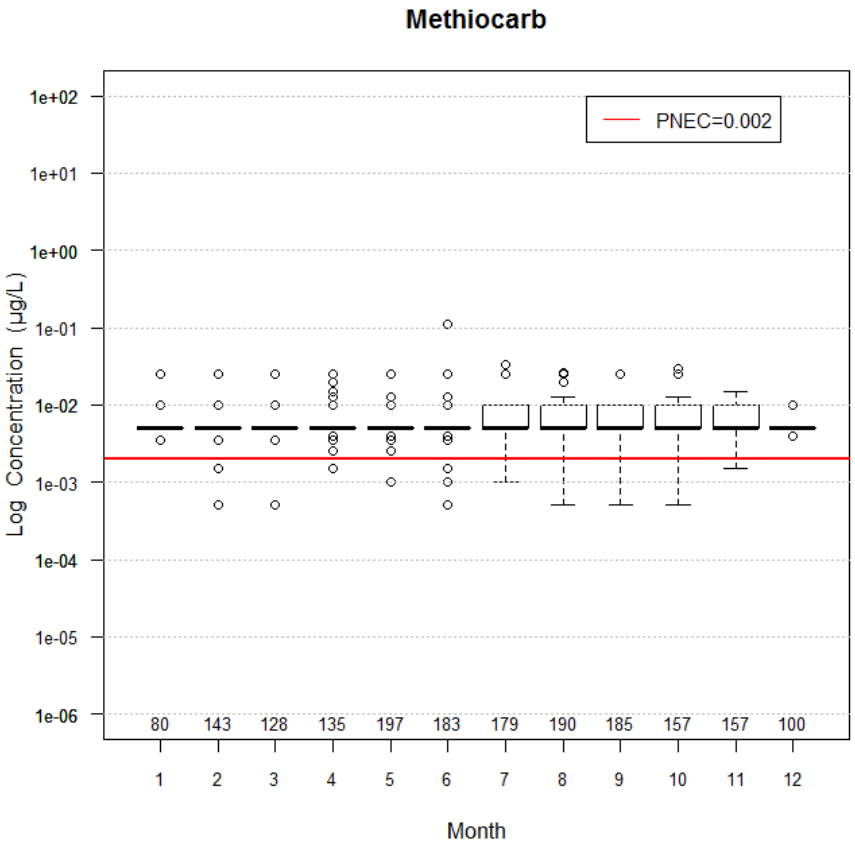

Estrone
PNEC=0.0036
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
6 8 15 3 115 93 8 7 18 26 39 2 10 4 35 4 4 4 12 134 13 10 4
#01 #02 #03 #05 #06 #07 #08 #09 #11 #12 #13 #15 #16 #17 #19 #20 #21 #22 #24 #26 #29 #30 #31
Country

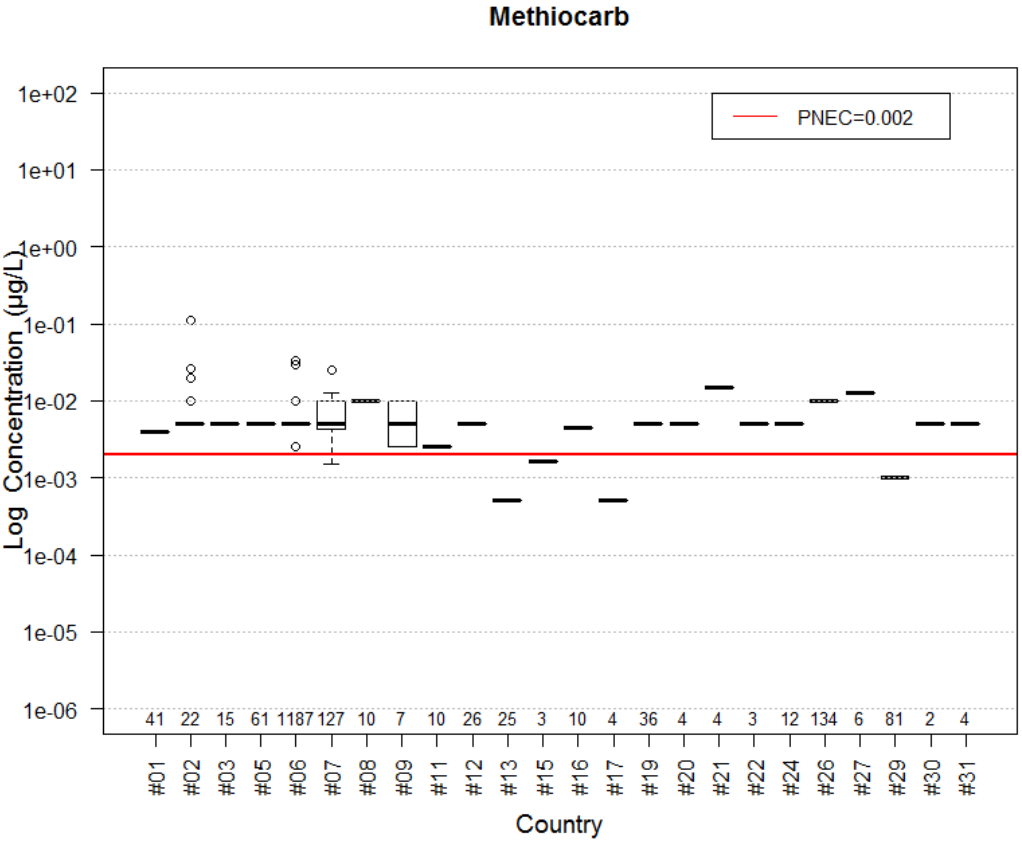
Imidacloprid





Methiocarb


Methiocarb
PNEC=0.002
Log Concentration (µg/L)
1e+02
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
80 143 128 135 197 183 179 190 185 157 157 100
1 2 3 4 5 6 7 8 9 10 11 12
Month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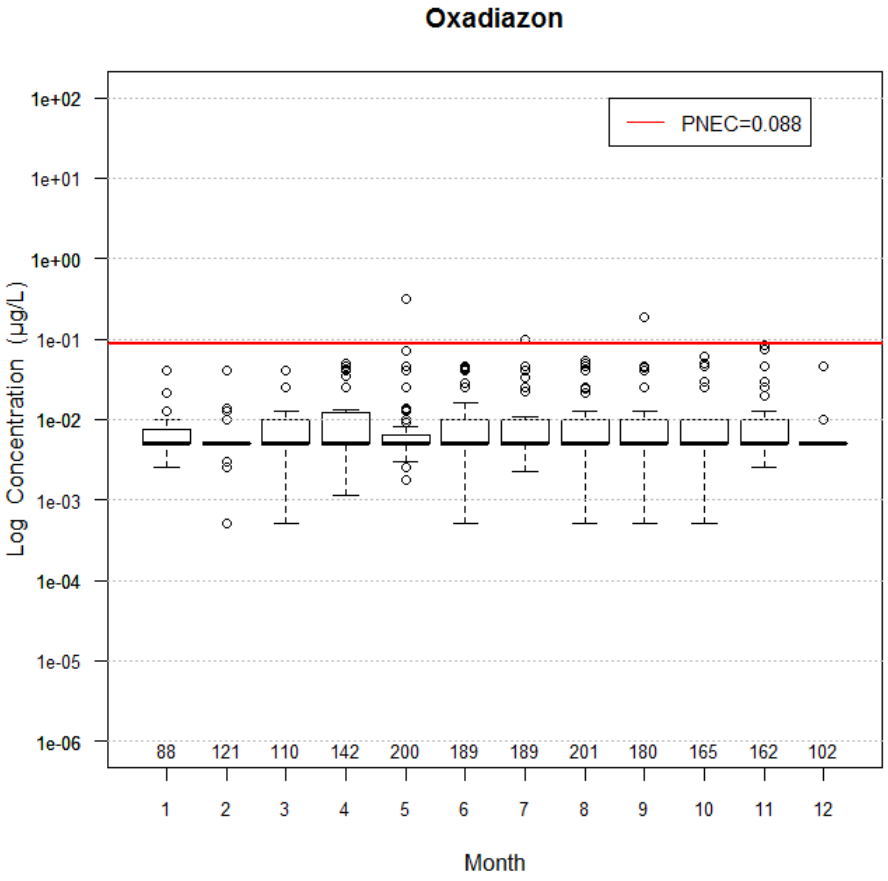
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
41 22 15 61 1187 127 10 7 10 26 25 3 10 4 36 4 4 3 12 134 6 81 2 4
#01 #02 #03 #05 #06 #07 #08 #09 #11 #12 #13 #15 #16 #17 #19 #20 #21 #22 #24 #26 #27 #29 #30 #31
Country

Oxadiazon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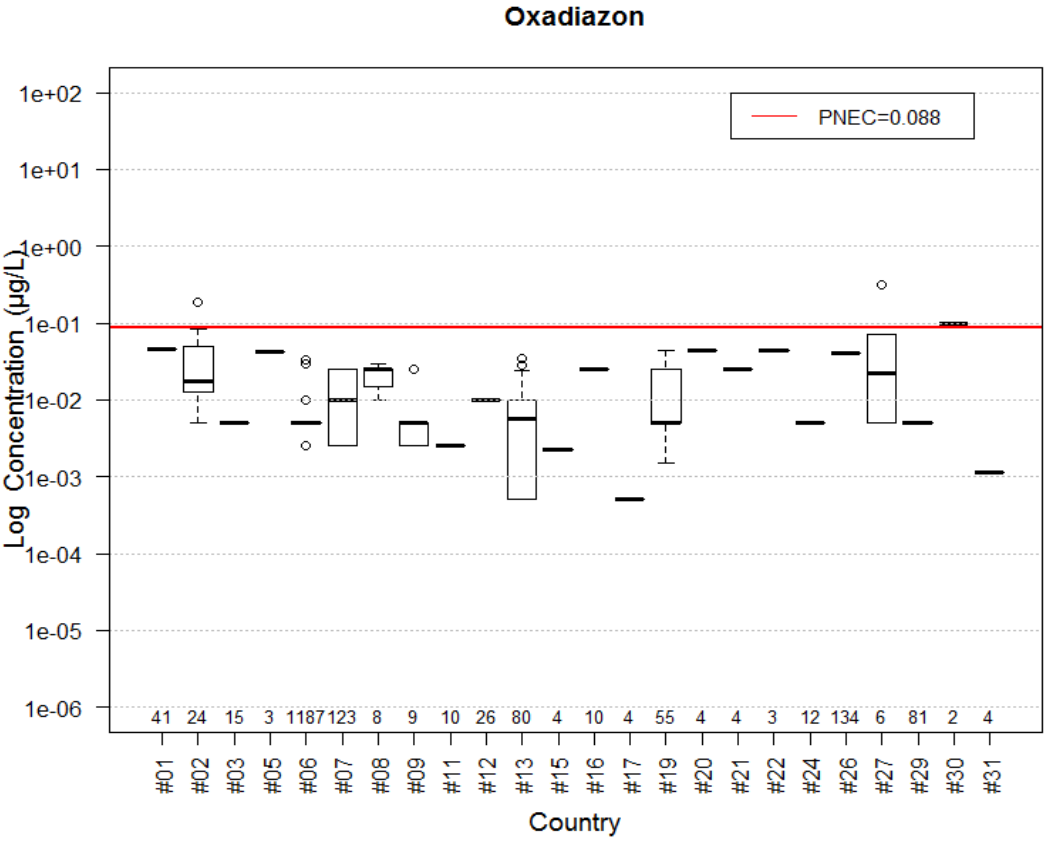
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
88 121 110 142 200 189 189 201 180 165 162 102
1 2 3 4 5 6 7 8 9 10 11 12
Month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1e+01
1e+00
1e-01
1e-02
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1e-04
1e-05
1e-06
41 24 15 3 1187 123 8 9 10 26 80 4 10 4 55 4 4 3 12 134 6 81 2 4
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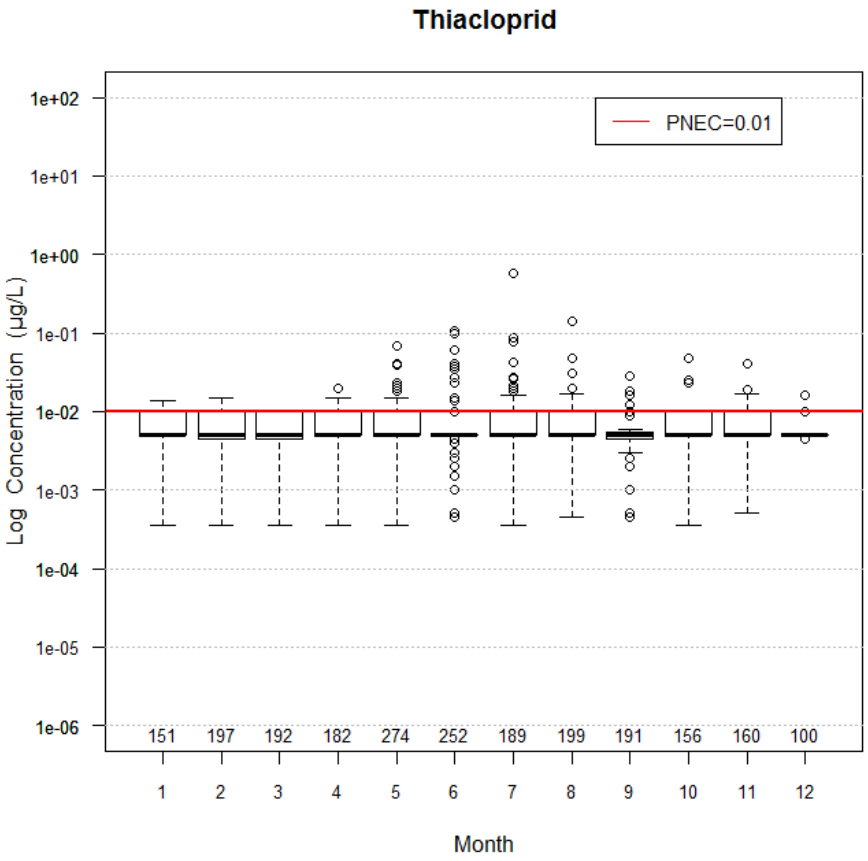
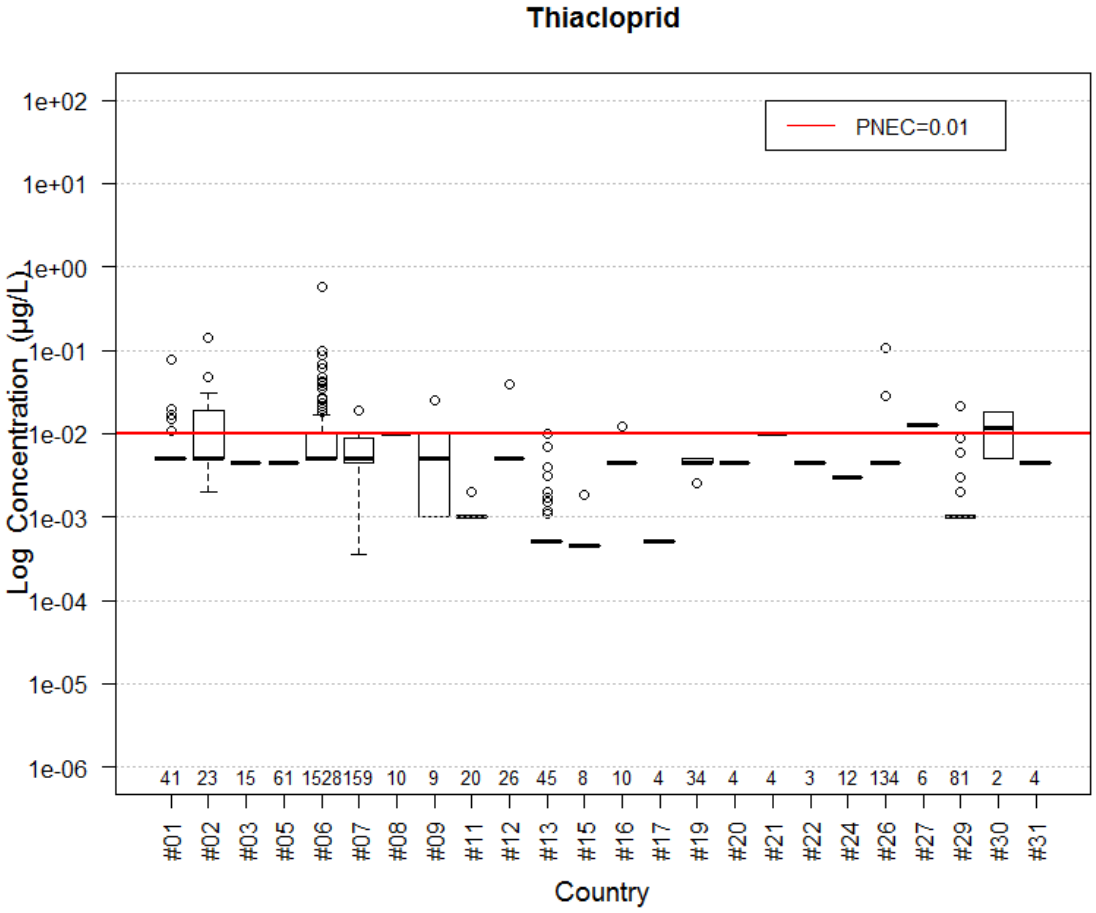
Country

Thiacloprid

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1e-04
1e-05
1e-06
41 23 15 61 1528 159 10 9 20 26 45 8 10 4 34 4 4 3 12 134 6 81 2 4
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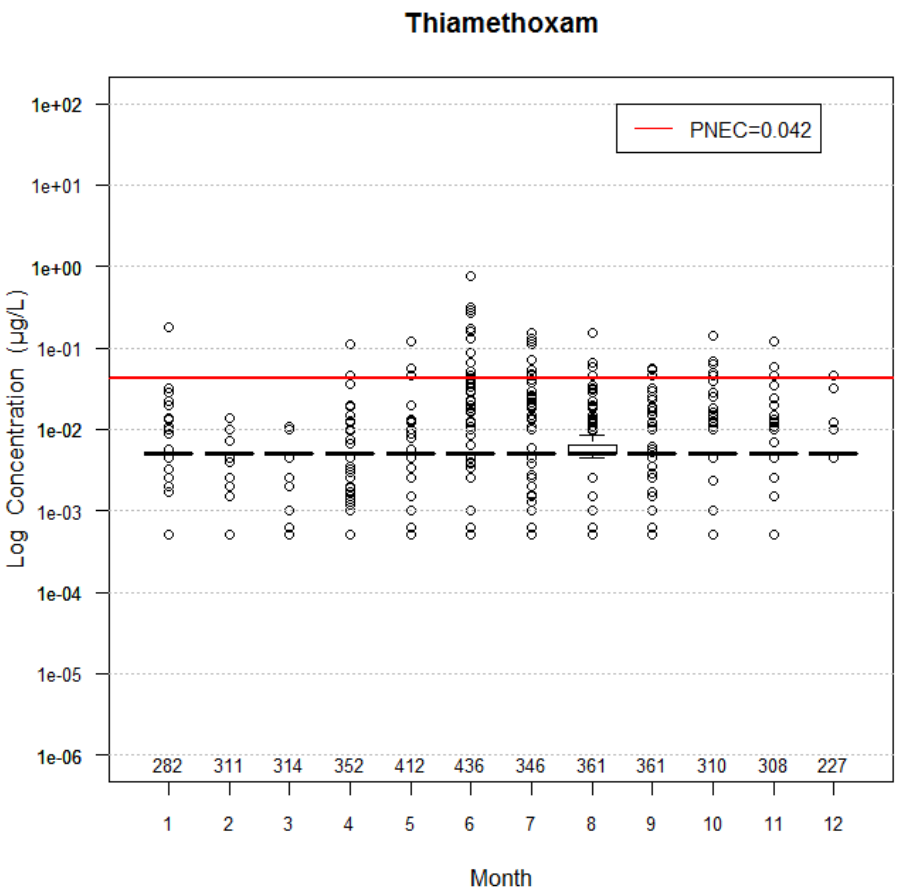
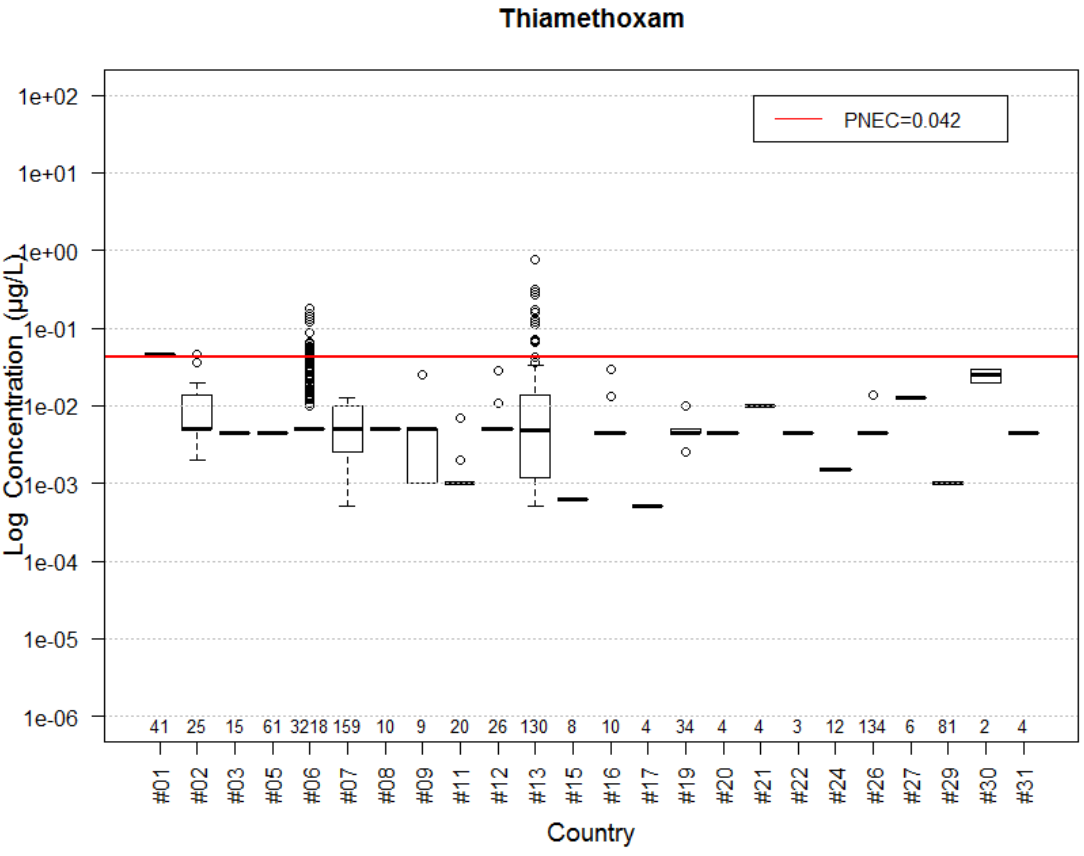
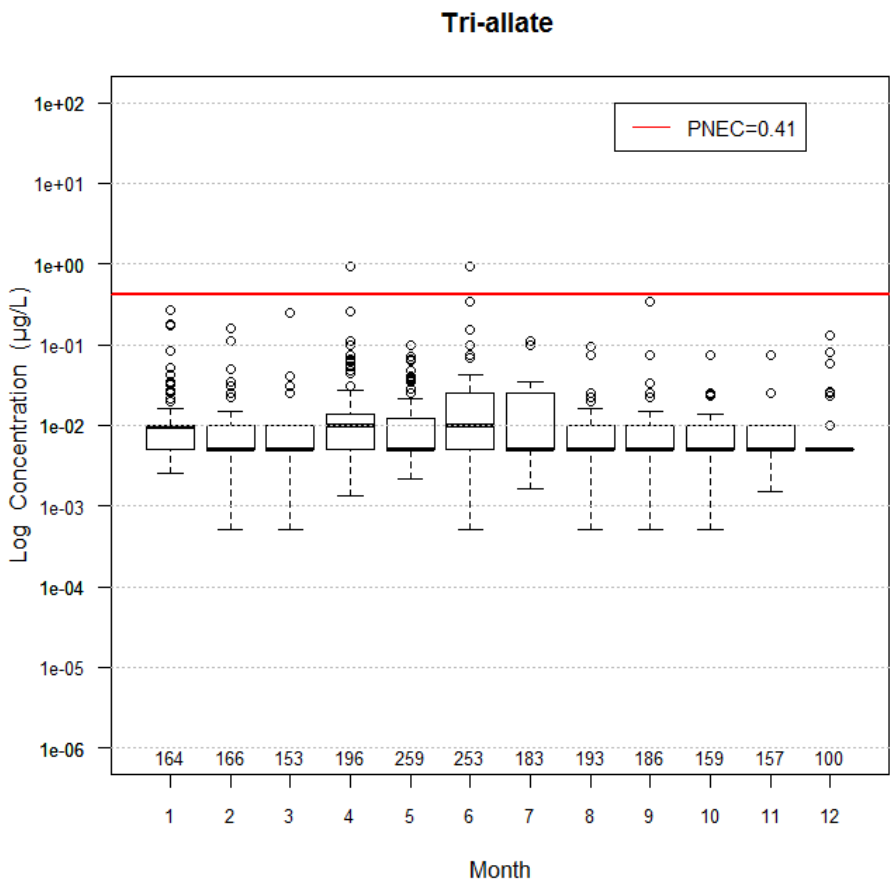
Country

Thiamethoxam





Tri-allate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1e+01
1e+00
1e-01
1e-02
1e-03
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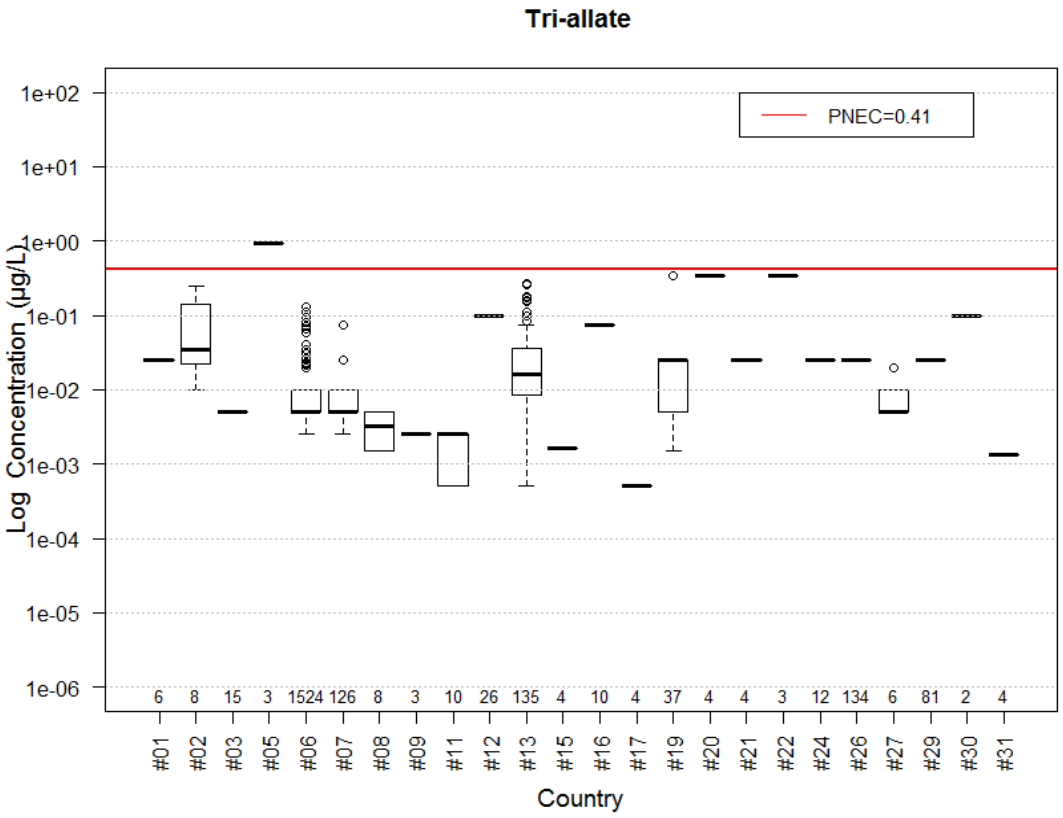
164 166 153 196 259 253 183 193 186 159 157 100
1 2 3 4 5 6 7 8 9 10 11 12
Month


Tri-allate
PNEC=0.41
Log Concentration (µg/L)
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1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
1e-05
1e-06
6 8 15 3 1524 126 8 3 10 26 135 4 10 4 37 4 4 3 12 134 6 81 2 4
#01 #02 #03 #05 #06 #07 #08 #09 #11 #12 #13 #15 #16 #17 #19 #20 #21 #22 #24 #26 #27 #29 #30 #31
Country

Annex 8: Evaluation of WL susbtances by the combined dataset

In addition to the WL dataset, the WL substances have been evaluated by a so-called "combined dataset", which is a combination of measurements from the monitoring prioritisation exercise (Carvalho et al., 2016) and the first year of WL monitoring.

WL dataset is unique and very useful since it includes a good quality data from all MS. However, the information provided by WL dataset is timely (only one year) and spatially (a few selected sampling stations) restricted. For this reason the WL substances also were evaluated additionally combining the WL dataset and the dataset used in the monitoring prioritisation exercise. The later does not necessarily include samples from all MS but has the advantage to cover a wider time period (2006-2014). Of course, the eventual duplicates were eliminated from the combined dataset.

The report is showing the results for the WL and combined datasets separately, so the experts could see the assessment of WL substances taking into account different spatial and temporal perspectives.

The combined dataset contains more data and covers a longer time period (2006-2016); it includes measurements from 26 countries and a total number of 232486 samples in Sc2 for the WL substances. After the application of the PNEC quality criterion to the records in Sc2 the total amount of samples is reduced by 28.6% to 166073 samples in Sc3 (related to the updated PNECs). The average percentage of quantification frequency is 20% (range 0.9%-73.2%) for data of Sc3.

All WL substances showed in Sc3 (related to the updated PNECs) a good quality of non-quantified samples except for 5 substances (EE2, E2, azithromycin, imidacloprid and methiocarb) that have a reduced quality of data but a sufficient amount of samples for making statistical analyses and to run the STE tool. These substances are identical to those already identified in the WL dataset.

The highest STE scores obtained by the combined dataset in Sc3 and updated PNECs were for: imidacloprid (1.30), methiocarb (1.23), azithromycin (1.22), diclofenac (1.22), 17-alpha-ethinylestradiol (0.86), 17-beta-estradiol (0.83), estrone (0.52), and clarithromycin (0.41).

The combined dataset in Sc3 and the updated PNECs give, in particular for the substances with higher scoring, slightly elevated scores in comparison to the WL dataset since the higher concentrations measured earlier than 2014-2015 (for details see Annex 8.2). Also worth to mention that the intermediate scored substances, including diclofenac and EE2 (with STE scores about 0.9), have relatively high risk quotients (above 5).

Annex 8.1 Concentrations of WL substances by the combined dataset

Next table gives a summary of the concentration statistics for the WL substances from the combined data set (all data scenarios) and updated PNECs.

In this case, the median of EE2 is exceeded PNEC only in Sc1. However, additional PNEC exceedances are observed for E2 (Sc1 and Sc2), diclofenac (Sc1), azithromycin (all scenarios), and methiocarb (Sc1 and Sc2).

Table: Summary statistics of concentrations for the WL substances (µg/l) considering the combined data set (all data scenarios) and updated PNECs. In bold the PNEC exceedance of the median concentration.

Substance	Scenario	Samples	PNEC	Median	Mean	P95	Max
	Sc1	86		**0.00011**	0.00024	0.00087	0.0030
17-alpha-Ethinylestradiol	Sc2	738	0.000035	0.000021	0.00045	0.0010	0.0125
	Sc3	469		0.000015	0.000053	0.00021	0.0030
	Sc1	140		**0.00041**	0.0011	0.0051	0.015
	Sc2	1767	0.0004	**0.00050**	0.00054	0.0010	0.015
17-beta-Estradiol	Sc3	716		0.00015	0.00031	0.0010	0.015
	Sc1	374		0.00085	0.0040	0.030	0.099
	Sc2	1358	0.0036	0.0025	0.0029	0.00566	0.099
Estrone	Sc3	1314		0.0025	0.0024	0.0050	0.099
	Sc1	12988		**0.069**	0.15	0.56	7.1
	Sc2	17748	0.05	0.040	0.11	0.46	7.1
Diclofenac	Sc3	17748		0.040	0.11	0.46	7.1
	Sc1	91		0.047	1.22	4.9	49.0
2,6-Di-tert-butyl-4-methylphenol	Sc2	1296	3.16	0.015	0.161	0.250	49.0
	Sc3	1293		0.015	0.151	0.250	49.0
	Sc1	116		0.305	0.420	1.4	1.8
2-Ethylhexyl-4-methoxycinnamate	Sc2	546	6.0	0.050	0.367	3.0	9.0
	Sc3	543		0.050	0.319	3.0	3.0
	Sc1	1144		0.030	0.050	0.150	1.1
	Sc2	6313	0.2	0.010	0.017	0.050	1.1
Erythromycin	Sc3	6313		0.010	0.017	0.050	1.1
	Sc1	3585		0.033	0.063	0.21	1.6
	Sc2	7443	0.12	0.015	0.036	0.13	1.6
Clarithromycin	Sc3	7443		0.015	0.036	0.13	1.6
	Sc1	410		**0.050**	0.088	0.31	1.0
	Sc2	2212	0.019	**0.025**	0.034	0.10	5.0
Azithromycin	Sc3	2210		**0.025**	0.030	0.10	1.0
	Sc1	377		**0.010**	0.031	0.098	0.96
	Sc2	24375	0.002	**0.010**	0.011	0.025	0.96
Methiocarb	Sc3	2781		0.001	0.006	0.010	0.96
	Sc1	8689		**0.034**	0.564	0.840	450.0
	Sc2	66827	0.0083	**0.010**	0.086	0.070	450.0
Imidacloprid	Sc3	24745		0.005	0.201	0.230	450.0
	Sc1	452		0.013	0.032	0.118	0.81
	Sc2	8623	0.01	0.005	0.008	0.010	0.81
Thiacloprid	Sc3	8533		0.005	0.008	0.010	0.81
	Sc1	538		0.028	0.062	0.190	3.18
	Sc2	9082	0.042	0.005	0.011	0.017	3.18
Thiamethoxam	Sc3	9082		0.005	0.011	0.017	3.18
	Sc1	315		0.014	0.037	0.140	0.78
	Sc2	5952	0.13	0.010	0.012	0.025	0.78
Clothianidin	Sc3	5952		0.010	0.012	0.025	0.78
	Sc1	65		0.020	0.022	0.046	0.074
	Sc2	7121	0.5	0.005	0.007	0.010	0.15
Acetamiprid	Sc3	7121		0.005	0.007	0.010	0.15
	Sc1	3071		0.020	3.5	26.0	270.0
	Sc2	50357	0.088	0.010	0.282	0.025	270.0
Oxadiazon	Sc3	50148		0.010	0.225	0.025	270.0
	Sc1	209		0.018	0.035	0.125	0.27
	Sc2	20728	0.41	0.020	0.016	0.025	0.95
Triallate	Sc3	20725		0.020	0.016	0.025	0.34

The following figure shows a box-whisker plot for the concentrations of samples for Sc3 of the combined dataset for each substance in comparison to the updated PNEC values. The lowermost line of the figure indicates the total number of samples per substance. Attention should be paid to the increased number of samples in the combined dataset.

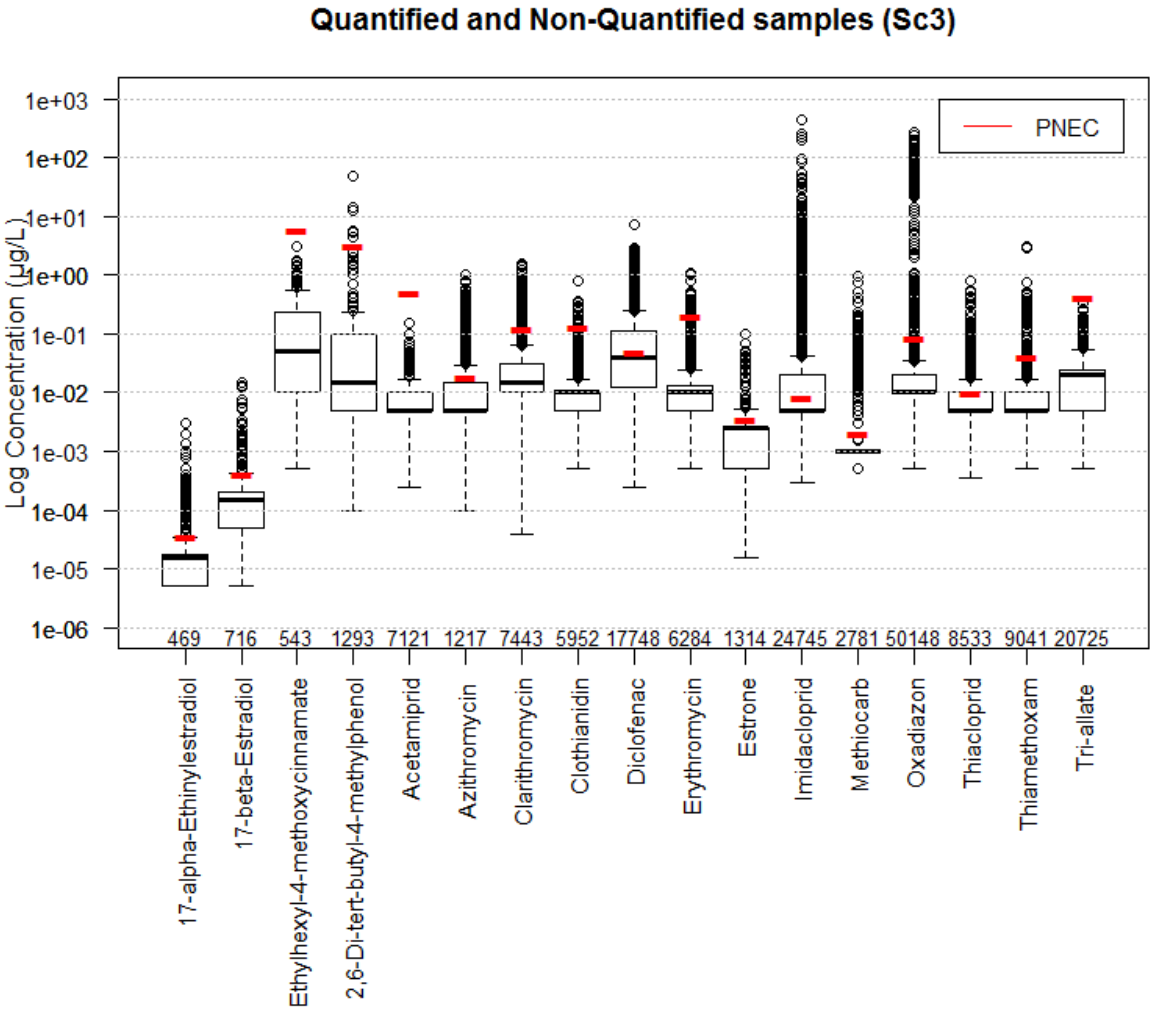


Figure: Box-plot of concentrations for combined dataset in Sc3 comparing to the updated PNEC values. The lowermost line of the figure indicates the total number of samples per substance.

The box-whisker plots of concentrations of WL substances for Sc2 and Sc1 scenarios of the combined data are given in the Annex 8.3. This annex also presents analyses for the quality of monitoring samples in the combined dataset.

Conclusions:

The European median surface water concentration of EE2 is exceeding its PNEC (0.035 ng/L) only in Sc1 (0.11 ng/L). For E2 the PNEC (0.40 ng/L) exceedance is found for the median concentration in Sc1 (0.41ng/L) and Sc2 (0.050 ng/L) but not in Sc3.

The median concentration of imidacloprid (0.018 µg/L) exceeds its PNEC (0.009 µg/L) in Sc1 (0.018 µg/L) and Sc2 (0.010 µg/L) but not in Sc3.

For diclofenac the median concentration exceeds its PNEC (0.05 µg/L) only in Sc1 (0.069 µg/L).

For azithromycin the median concentration exceeds its PNEC (0.019 µg/L) in all scenarios, Sc1 (0.050 µg/L) and both Sc3 and Sc2 (0.025 µg/L) respectively.

The median concentration of methiocarb exceeds its PNEC concentration (0.002 µg/L) only in Sc1 and Sc2 (for both 0.010 µg/L).

Annex 8.2 Detailed statistics for WL substances by the combined dataset (Sc3 is based on the updated PNECs).

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
17-alpha-Ethinylestradiol	3.50E-05	Sc2	25	272	738	652	11.65	5.00E-06	4.50E-04	1.58E-03	2.13E-05	1.00E-03	1.00E-03	1.25E-02
		Sc1	10	57	86	0	100	3.00E-05	2.37E-04	4.25E-04	1.05E-04	3.75E-04	8.70E-04	3.00E-03
		Sc3	14	162	469	383	18.34	5.00E-06	5.34E-05	2.01E-04	1.50E-05	9.30E-05	2.05E-04	3.00E-03
17-beta-Estradiol	4.00E-04	Sc2	25	459	1767	1627	7.92	5.00E-06	5.41E-04	1.21E-03	5.00E-04	5.00E-04	1.00E-03	1.50E-02
		Sc1	13	90	140	0	100	4.28E-05	1.13E-03	2.22E-03	4.10E-04	2.02E-03	5.12E-03	1.50E-02
		Sc3	20	262	716	576	19.55	5.00E-06	3.09E-04	1.06E-03	1.50E-04	4.00E-04	1.00E-03	1.50E-02
2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Sc2	24	261	1296	1205	7.02	1.00E-04	1.61E-01	1.51E+00	1.50E-02	1.25E-01	2.50E-01	4.90E+01
		Sc1	7	35	91	0	100	6.66E-03	1.22E+00	5.51E+00	4.70E-02	1.80E+00	4.87E+00	4.90E+01
		Sc3	23	258	1293	1202	7.04	1.00E-04	1.51E-01	1.49E+00	1.50E-02	1.25E-01	2.50E-01	4.90E+01
2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sc2	24	201	546	430	21.25	5.00E-04	3.67E-01	9.72E-01	5.00E-02	7.55E-01	3.00E+00	9.00E+00
		Sc1	6	19	116	0	100	3.00E-03	4.20E-01	4.05E-01	3.05E-01	1.00E+00	1.40E+00	1.80E+00
		Sc3	23	198	543	427	21.36	5.00E-04	3.19E-01	7.32E-01	5.00E-02	7.50E-01	3.00E+00	3.00E+00
Acetamiprid	5.00E-01	Sc2	24	750	7121	7056	0.91	2.50E-04	6.54E-03	5.00E-03	5.00E-03	1.00E-02	1.00E-02	1.50E-01
		Sc1	8	31	65	0	100	1.37E-03	2.17E-02	1.53E-02	2.00E-02	4.02E-02	4.60E-02	7.40E-02
		Sc3	24	750	7121	7056	0.91	2.50E-04	6.54E-03	5.00E-03	5.00E-03	1.00E-02	1.00E-02	1.50E-01
Azithromycin	1.90E-02	Sc2	25	336	2212	1802	18.54	1.00E-04	3.44E-02	1.61E-01	2.50E-02	5.00E-02	1.00E-01	5.00E+00
		Sc1	17	105	410	0	100	2.00E-04	8.83E-02	1.20E-01	5.00E-02	2.20E-01	3.11E-01	1.00E+00
		Sc3	20	230	1217	807	33.69	1.00E-04	3.32E-02	8.00E-02	5.00E-03	9.00E-02	1.70E-01	1.00E+00
Clarithromycin	1.20E-01	Sc2	25	733	7443	3858	48.17	3.80E-05	3.63E-02	7.73E-02	1.50E-02	7.50E-02	1.30E-01	1.60E+00
		Sc1	18	483	3585	0	100	3.80E-05	6.28E-02	1.05E-01	3.30E-02	1.30E-01	2.10E-01	1.60E+00

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
		Sc3	25	733	7443	3858	48.17	3.80E-05	3.63E-02	7.73E-02	1.50E-02	7.50E-02	1.30E-01	1.60E+00
Clothianidin	1.30E-01	Sc2	24	607	5952	5637	5.29	5.00E-04	1.18E-02	1.90E-02	1.00E-02	2.50E-02	2.50E-02	7.80E-01
		Sc1	7	91	315	0	100	7.00E-04	3.72E-02	7.05E-02	1.40E-02	8.92E-02	1.40E-01	7.80E-01
		Sc3	24	607	5952	5637	5.29	5.00E-04	1.18E-02	1.90E-02	1.00E-02	2.50E-02	2.50E-02	7.80E-01
Diclofenac	5.00E-02	Sc2	26	1340	17748	4760	73.18	2.50E-04	1.10E-01	2.07E-01	4.00E-02	2.80E-01	4.61E-01	7.10E+00
		Sc1	24	1149	12988	0	100	5.30E-04	1.47E-01	2.31E-01	6.90E-02	3.50E-01	5.60E-01	7.10E+00
		Sc3	26	1340	17748	4760	73.18	2.50E-04	1.10E-01	2.07E-01	4.00E-02	2.80E-01	4.61E-01	7.10E+00
Erythromycin	2.00E-01	Sc2	25	601	6313	5169	18.12	5.00E-04	1.72E-02	3.58E-02	1.00E-02	3.00E-02	5.00E-02	1.10E+00
		Sc1	13	263	1144	0	100	1.00E-03	4.99E-02	7.43E-02	3.00E-02	1.00E-01	1.50E-01	1.10E+00
		Sc3	25	601	6284	5140	18.20	5.00E-04	1.72E-02	3.58E-02	1.00E-02	3.00E-02	5.00E-02	1.10E+00
Estrone	3.60E-03	Sc2	24	452	1358	984	27.54	1.50E-05	2.88E-03	6.24E-03	2.50E-03	2.54E-03	5.66E-03	9.90E-02
		Sc1	16	182	374	0	100	3.97E-05	3.98E-03	1.02E-02	8.47E-04	5.16E-03	3.00E-02	9.90E-02
		Sc3	23	436	1314	940	28.46	1.50E-05	2.41E-03	5.57E-03	2.50E-03	2.50E-03	5.00E-03	9.90E-02
Imidacloprid	8.30E-03	Sc2	24	4925	66827	58138	13.00	3.00E-04	8.63E-02	3.29E+00	1.00E-02	3.00E-02	7.00E-02	4.50E+02
		Sc1	15	1758	8689	0	100	1.20E-03	5.64E-01	9.10E+00	3.40E-02	3.70E-01	8.40E-01	4.50E+02
		Sc3	22	2761	24745	16056	35.11	3.00E-04	2.01E-01	5.40E+00	5.00E-03	8.00E-02	2.30E-01	4.50E+02
Methiocarb	2.00E-03	Sc2	24	2746	24375	23998	1.55	5.00E-04	1.14E-02	1.46E-02	1.00E-02	2.50E-02	2.50E-02	9.60E-01
		Sc1	7	222	377	0	100	3.00E-03	3.11E-02	7.84E-02	1.00E-02	6.00E-02	9.76E-02	9.60E-01
		Sc3	10	554	2781	2404	13.56	5.00E-04	5.07E-03	3.06E-02	5.00E-03	8.00E-03	1.40E-02	9.60E-01
Oxadiazon	8.80E-02	Sc2	24	4108	50357	47286	6.10	5.00E-04	2.82E-01	4.44E+00	1.00E-02	2.50E-02	2.50E-02	2.70E+02
		Sc1	9	916	3071	0	100	1.80E-03	3.48E+00	1.71E+01	2.00E-02	2.70E-01	2.60E+01	2.70E+02
		Sc3	23	4106	50148	47077	6.12	5.00E-04	2.25E-01	4.31E+00	1.00E-02	2.50E-02	2.50E-02	2.70E+02
Thiacloprid	1.00E-02	Sc2	24	1085	8623	8171	5.24	3.50E-04	8.37E-03	1.73E-02	5.00E-03	1.00E-02	1.00E-02	8.13E-01
		Sc1	14	147	452	0	100	8.00E-04	3.20E-02	6.92E-02	1.30E-02	6.49E-02	1.18E-01	8.13E-01
		Sc3	23	1037	8533	8081	5.30	3.50E-04	8.09E-03	1.71E-02	5.00E-03	1.00E-02	1.00E-02	8.13E-01
Thiamethoxam	4.20E-02	Sc2	24	961	9082	8544	5.92	5.00E-04	1.08E-02	5.02E-02	5.00E-03	1.50E-02	1.69E-02	3.18E+00

Substance	PNEC (µg/L)	Scenario	Countries	Sites	Samples	Samples < LOQ	Quantified samples (%)	Min	Mean	SD	Median	P90	P95	Max
		Sc1	12	165	538	0	100	1.20E-03	6.17E-02	1.98E-01	2.80E-02	1.23E-01	1.90E-01	3.18E+00
		Sc3	24	955	9041	8503	5.95	5.00E-04	1.06E-02	5.02E-02	5.00E-03	1.50E-02	1.50E-02	3.18E+00
Tri-allate	4.10E-01	Sc2	24	2253	20728	20519	1.01	5.00E-04	1.60E-02	1.82E-02	2.00E-02	2.50E-02	2.50E-02	9.45E-01
		Sc1	6	65	209	0	100	2.20E-03	3.45E-02	4.43E-02	1.80E-02	7.78E-02	1.25E-01	2.70E-01
		Sc3	23	2250	20725	20516	1.01	5.00E-04	1.58E-02	1.44E-02	2.00E-02	2.50E-02	2.50E-02	3.35E-01

The figures in this annex give information for the quality of the combined monitoring dataset and presents the box-plots of concentrations together with the updated PNECs for the WL substances.

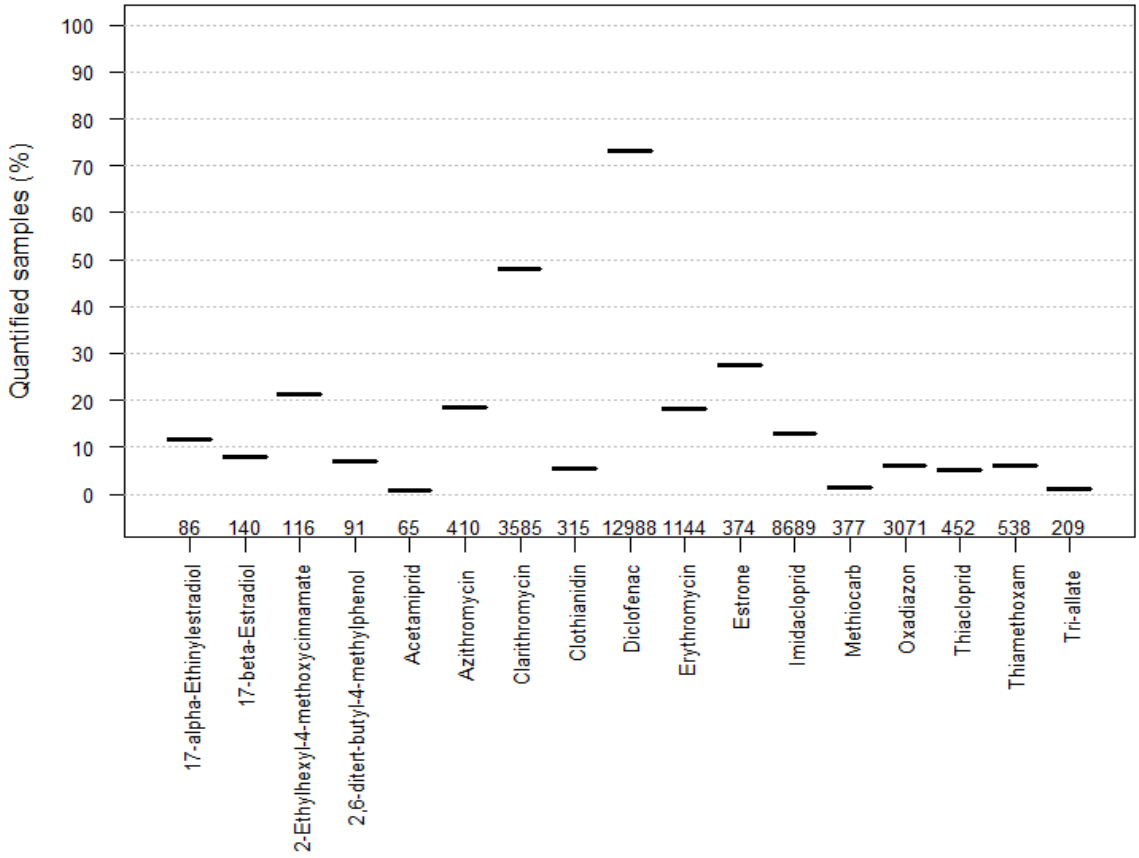


Figure: Percentage of quantified samples as a part from the total number of samples per substance for data in Sc2 of combined dataset. The amount of quantified samples per substance is given at the lowermost line of the figure. All WL substances have more than 51 quantified samples but 3 substances (17-alpha-Ethinylestradiol, 2,6-di-tert-butyl-4-methylphenol and acetamiprid) have less than 100.

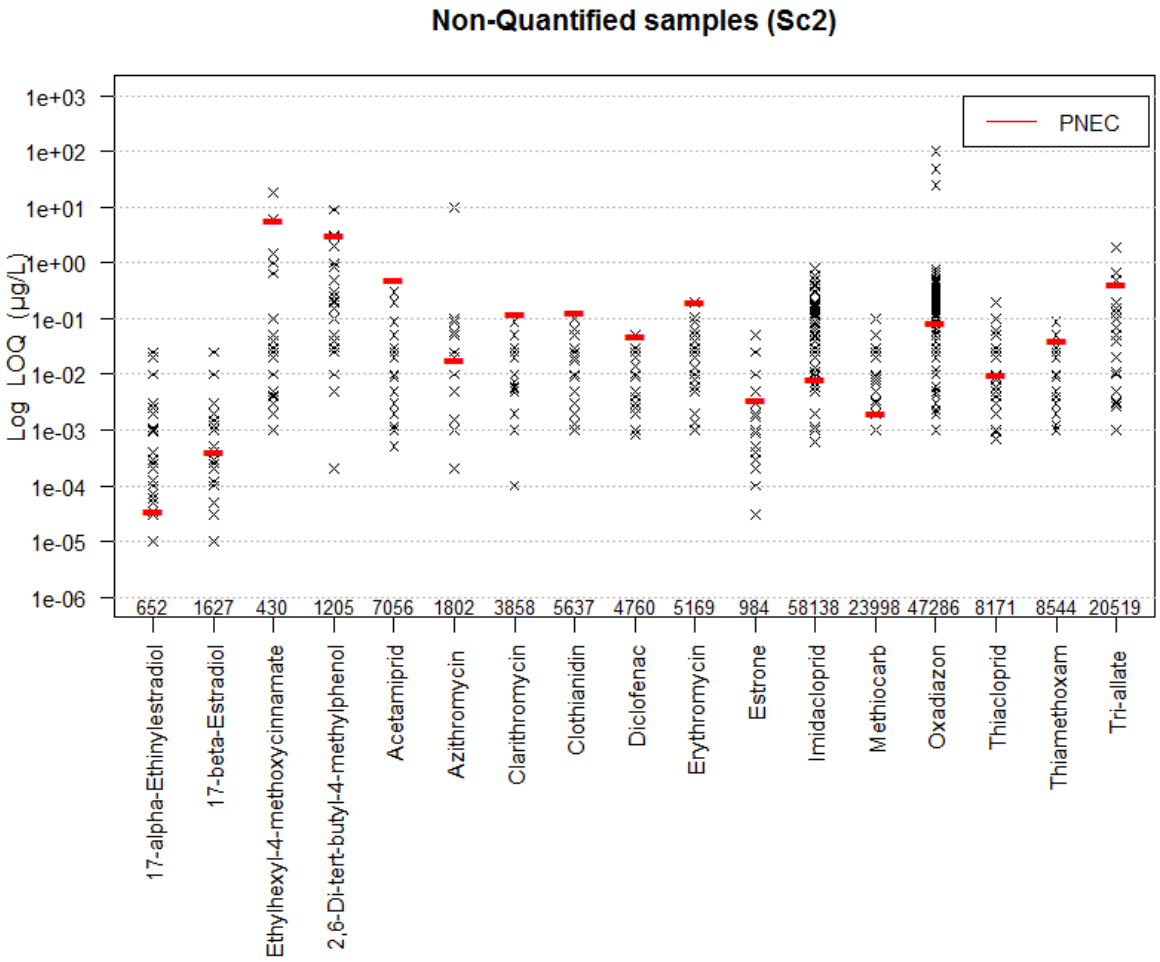


Figure: Range of LOQs for the non-quantified samples in the combined dataset per substance compared to the updated PNEC values. The amount of non-quantified samples per substance is given at the lowermost line of the figure.

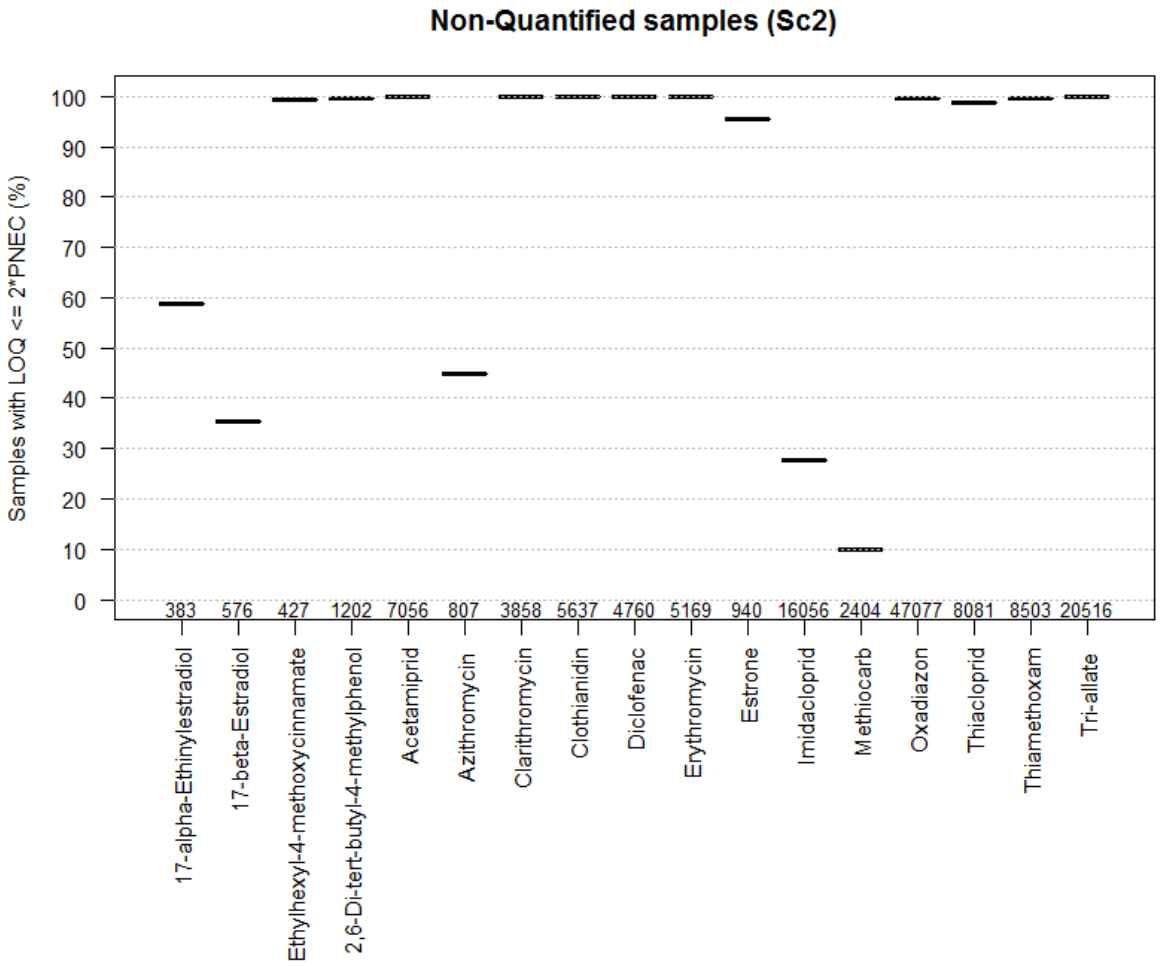


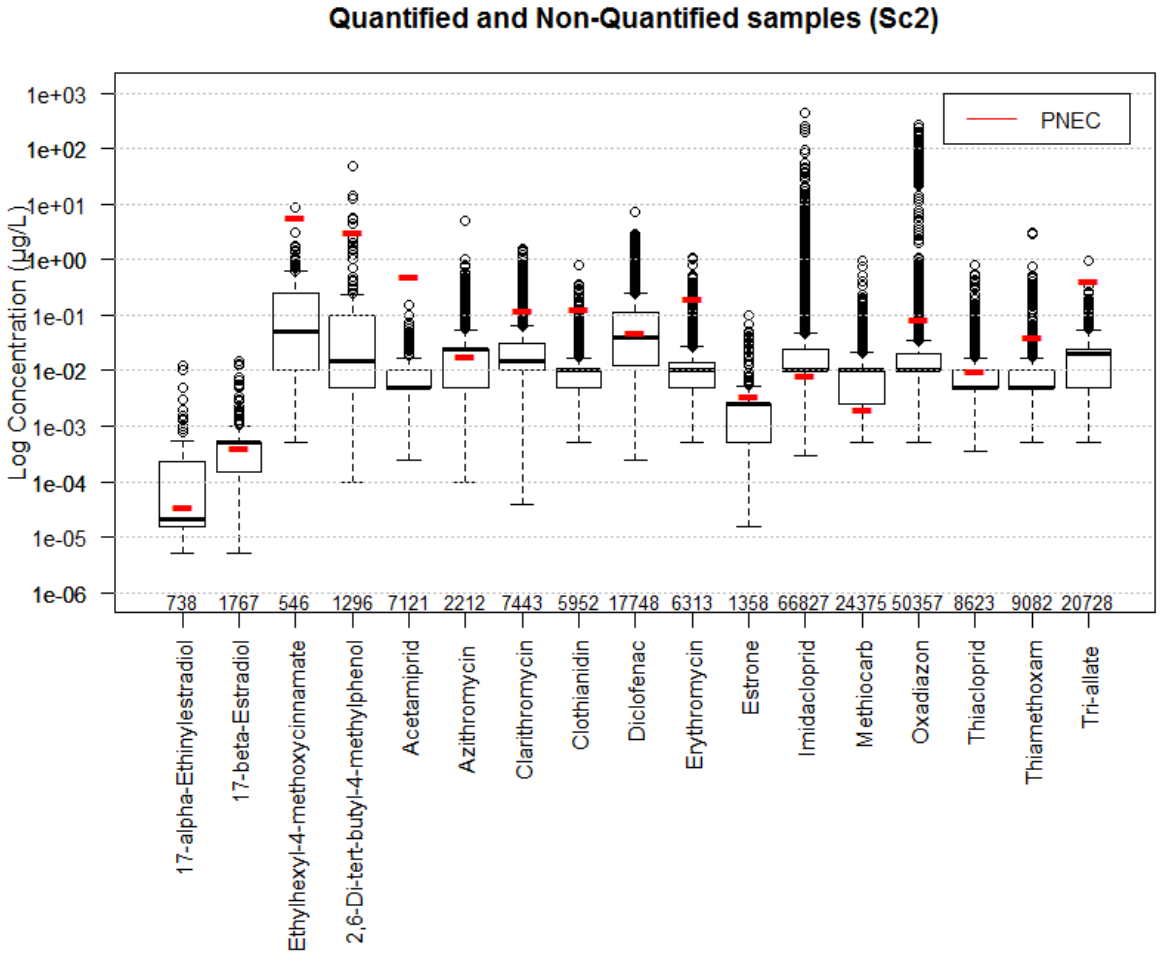
Figure: Percentage of non-quantified samples with 0.5*LOQ ≤ updated PNECs in Sc2 of combined dataset. The amount of these samples is given per each substance at the lowermost line of the figure. All WL substances showed a good quality of non-quantified samples in the combined dataset (except 17-alpha-Ethinylestradiol, 17-beta-Estradiol, Azithromycin, Imidacloprid and Methiocarb that have a reduced quality of data).

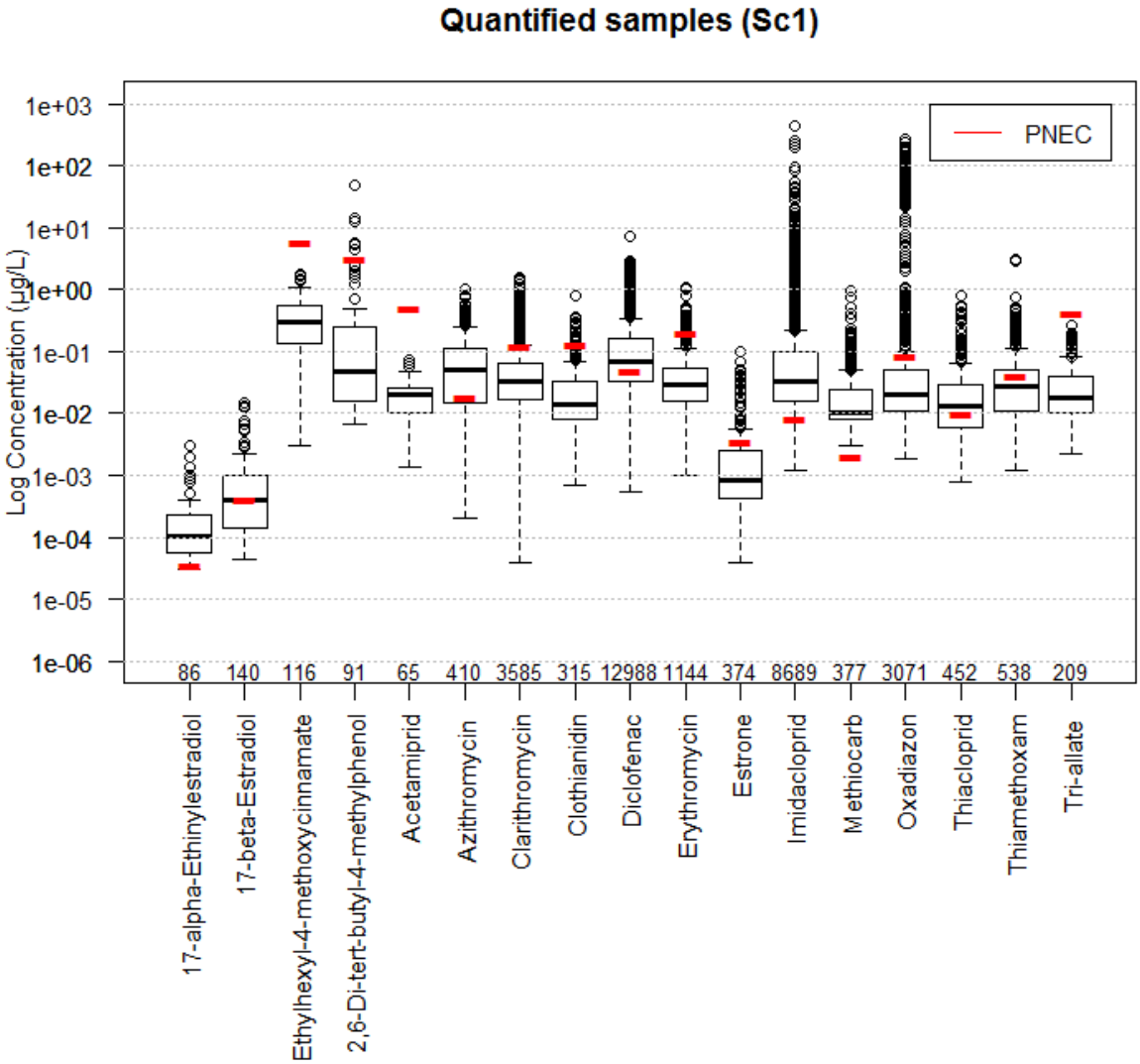
Conclusions (combined dataset and updated PNECs):

All WL substances have in Sc3 and Sc2 more than 51 quantified samples but 3 substances (17-alpha-Ethinylestradiol, 2,6-di-tert-butyl-4-methylphenol and acetamiprid) have less than 100 quantifed samples.

All WL substances showed in Sc3 and Sc2 a good quality of non-quantified samples in the combined dataset except 17-alpha-ethinylestradiol, 17-beta-estradiol, azithromycin, imidacloprid and methiocarb) that have a reduced quality of data but a sufficient amount of samples for making statistical analyses and to running the STE assessment tool.

The next two figures show for Sc2 and Sc1 of combined dataset the box-whisker plots for WL substances in comparison to the updated PNEC values. The concentrations of the non-quantified samples are set to LOQ/2. The lowermost line of the figure also indicates the total number of samples per substance.





Annex 8.3 STE scores of WL substances by the combined dataset

The detailed information about the STE scores calculated by the combined dataset and the updated PNECs for all data scenarios are presented in tabular form in Annex 8.4 This annex also shows the detailed specific information about the individual STE factors in Sc3 scenario.

The next figure displaces a graphical comparison of the STE scores for the combined monitoring dataset in Sc2 and Sc3 scenarios considering the updated PNECs (2-Ethylhexyl-4-methoxycinnamate is reported only in the WL). All scores of WL substances in Sc3 are below 1.4 and 4 substances (imidacloprid, methiocarb, azithromycin and diclofenac) showed intermediate range scores.

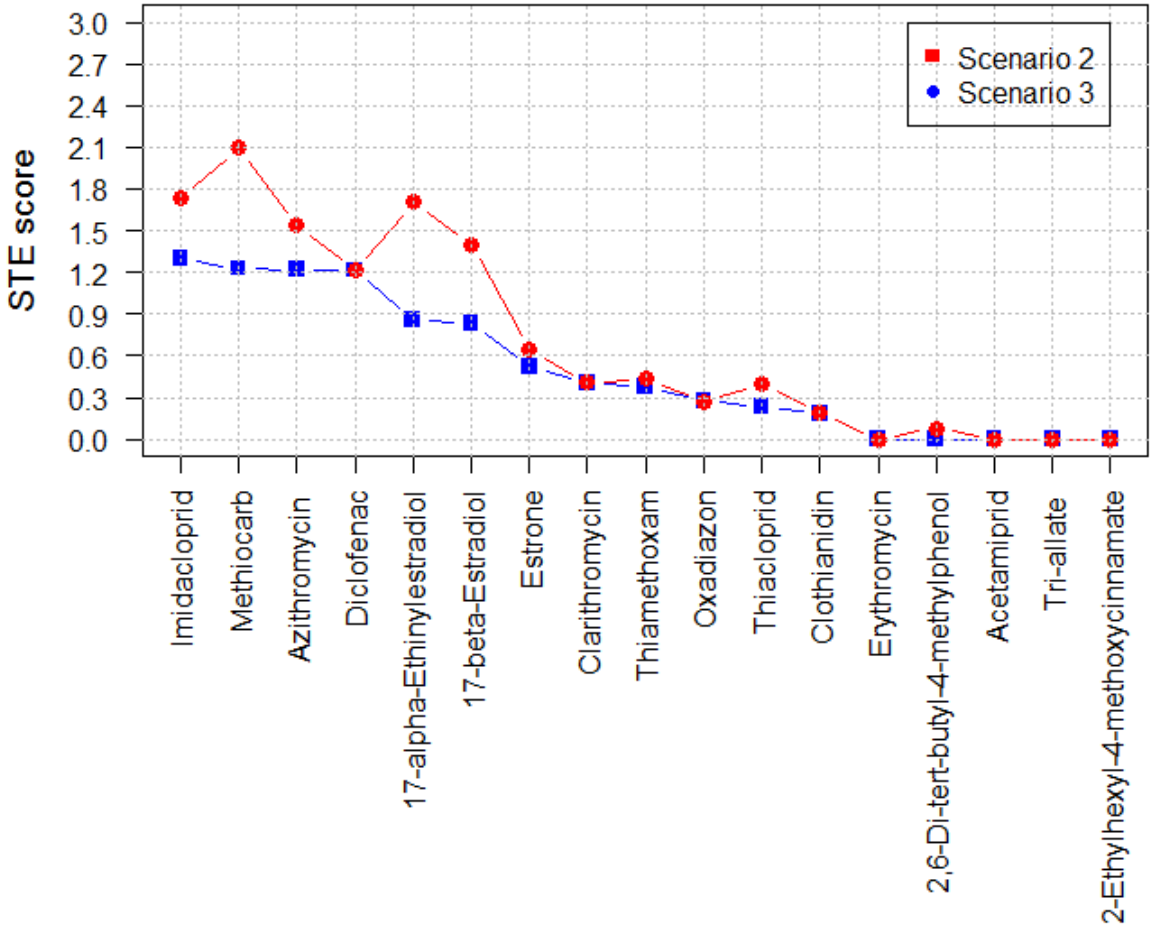


Figure: Comparison of STE scores obtained by combined dataset for Sc2 and Sc3 scenarios (2-ethylhexyl-4-methoxycinnamate is reported only in the WL dataset) considering the updated PNEC values.

The graphical comparison of the STE scores for the combined monitoring data in Sc1 and Sc3 scenarios and updated PNECs could be seen in Annex 8.4. Interestingly, in Sc1 three WL substances (imidacloprid, methiocarb and 17-alpha-ethinylestradiol) have very high or high STE scores (STE>2.2; for Sc2 these substances also obtained higher scores). The reason for the deviation between the scores in Sc3 and Sc1 could be the lower/reduced quality of the data for these substances, made available to the JRC in the prioritisation exercise.

Lastly, on the next figure could be seen the difference of STE scores for scenario Sc3 obtained when applying the updated PNECs either to the first WL dataset or to the combined one. The combined dataset gives, in particular for the substances with higher scores, slightly elevated results (since the higher concentrations measured earlier than 2014-2015; for details see Annex 8.3) but none of WL substances has high or very high STE score The lowermost line of the figure shows for information the RQ(P95) for the Sc3 of the combined dataset. Worth to mention that the intermediate scored substances by WL dataset, including diclofenac and EE2 (with STE scores about 0.9), have relatively high RQs (more than 5).

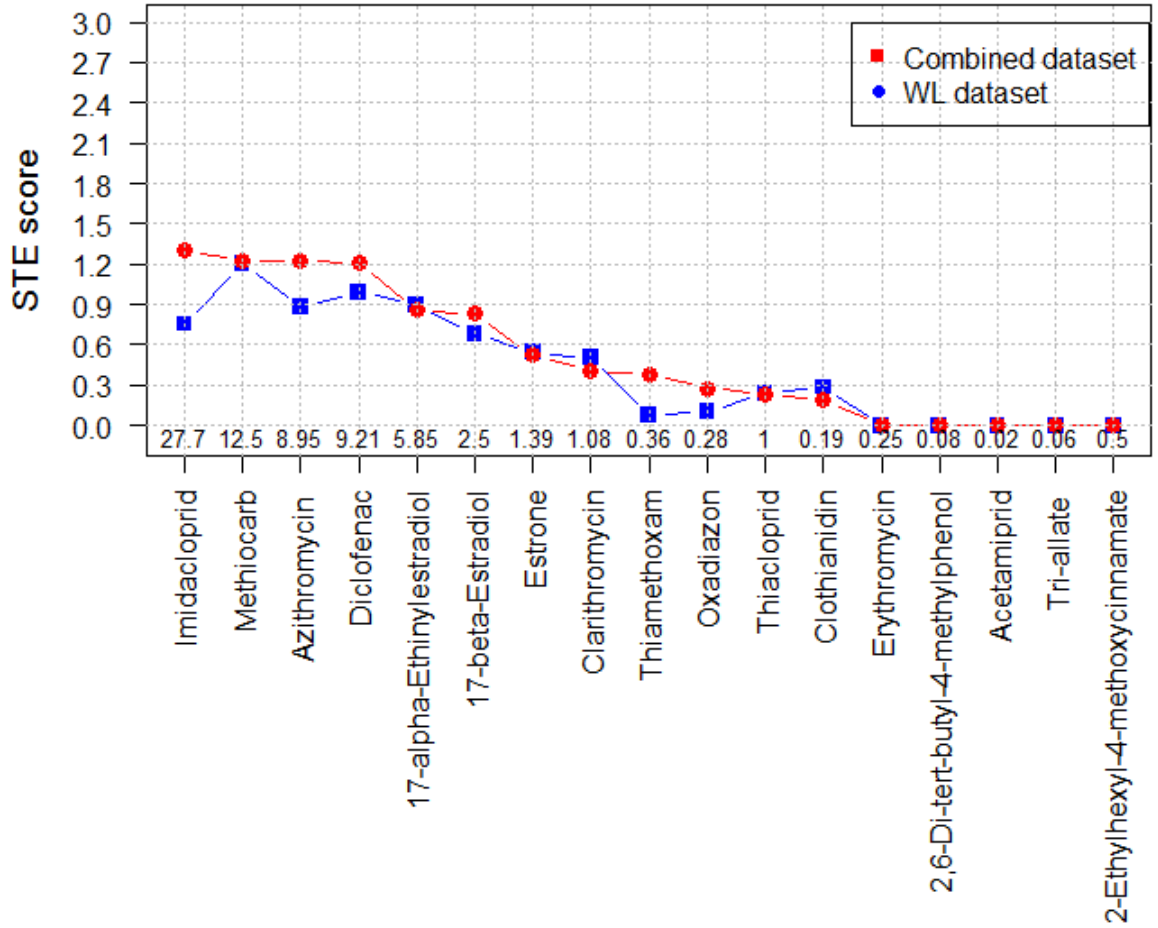


Figure: Comparison of STE scores obtained by different datasets (the first WL and the combined dataset) for data in Sc3 considering the updated PNEC values. The lowermost line shows the RQ(P95) for the Sc3 of the combined dataset.

Conclusions:

The combined dataset in Sc3 (first WL and prioritisation exercise) and updated PNECs showed STE scores below 1.4 and 4 substances (imidacloprid, methiocarb, azithromycin and diclofenac) have intermediate range scores.

The combined dataset in Sc3 and the updated PNECs give slightly elevated scores in comparison to the WL dataset since the higher concentrations measured earlier than 2014-2015. The intermediate scored substances by the WL dataset, including diclofenac and EE2 (with STE scores about 0.9), have relatively high RQs (more than 5).

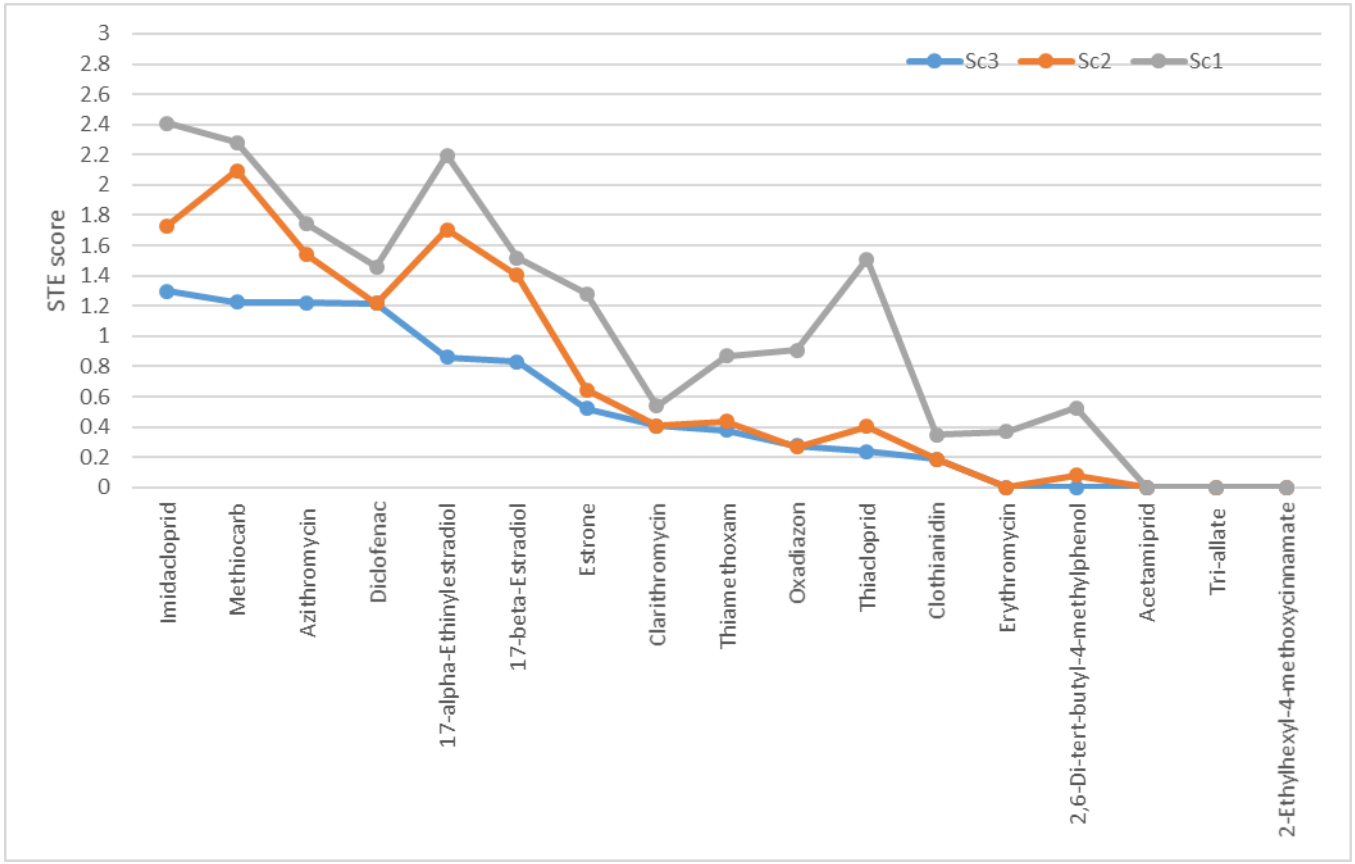
Annex 8.4 Detailed STE results by the combined dataset and updated PNECs: STE factors, STE scores and RQ(P95) (all data scenarios).

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
57-63-6	17-alpha-Ethinylestradiol	3.50E-05	Estrogen	Sc2	2.86E+01	5.03E-01	7.91E-01	4.10E-01	1.70E+00
				Sc1	2.49E+01	9.30E-01	9.86E-01	2.80E-01	2.20E+00
				Sc3	5.85E+00	2.16E-01	5.36E-01	1.10E-01	8.62E-01
50-28-2	17-beta-Estradiol	4.00E-04	Estrogen	Sc2	2.50E+00	3.28E-01	9.64E-01	1.10E-01	1.40E+00
				Sc1	1.28E+01	4.79E-01	8.60E-01	1.80E-01	1.52E+00
				Sc3	2.50E+00	8.76E-02	6.72E-01	7.00E-02	8.29E-01
128-37-0	2,6-Di-tert-butyl-4-methylphenol	3.16E+00	Antioxidant	Sc2	7.91E-02	7.98E-04	7.89E-02	0.00E+00	7.97E-02
				Sc1	1.54E+00	2.04E-02	4.33E-01	7.00E-02	5.24E-01
				Sc3	7.91E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5466-77-3	2-Ethylhexyl-4-methoxycinnamate	6.00E+00	Sunscreen	Sc2	5.00E-01	6.22E-04	0.00E+00	0.00E+00	6.22E-04
				Sc1	2.33E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	5.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
135410-20-7	Acetamiprid	5.00E-01	Neonicotinoid Insecticide	Sc2	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	9.20E-02	0	0	0	0
				Sc3	2.00E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
83905-01-5	Azithromycin	1.90E-02	Antibiotic	Sc2	5.26E+00	4.45E-01	9.12E-01	1.80E-01	1.54E+00
				Sc1	1.64E+01	5.61E-01	8.99E-01	2.80E-01	1.74E+00
				Sc3	8.95E+00	2.06E-01	8.33E-01	1.80E-01	1.22E+00
81103-11-9	Clarithromycin	1.20E-01	Antibiotic	Sc2	1.08E+00	2.40E-02	3.42E-01	4.00E-02	4.06E-01
				Sc1	1.75E+00	7.57E-02	3.94E-01	7.00E-02	5.40E-01

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
				Sc3	1.08E+00	2.40E-02	3.42E-01	4.00E-02	4.06E-01
210880-92-5	Clothianidin	1.30E-01	Neonicotinoid Insecticide	Sc2	1.92E-01	1.37E-04	1.88E-01	0.00E+00	1.88E-01
				Sc1	1.08E+00	1.57E-02	2.90E-01	4.00E-02	3.46E-01
				Sc3	1.92E-01	1.37E-04	1.88E-01	0.00E+00	1.88E-01
15307-86-5	Diclofenac	5.00E-02	Analgesic	Sc2	9.21E+00	4.43E-01	5.92E-01	1.80E-01	1.22E+00
				Sc1	1.12E+01	6.03E-01	6.76E-01	1.80E-01	1.46E+00
				Sc3	9.21E+00	4.43E-01	5.92E-01	1.80E-01	1.22E+00
114-07-8	Erythromycin	2.00E-01	Antibiotic	Sc2	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc1	7.50E-01	1.29E-02	3.15E-01	4.00E-02	3.68E-01
				Sc3	2.50E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
53-16-7	Estrone	3.60E-03	Estrogen	Sc2	1.57E+00	6.69E-02	4.68E-01	1.10E-01	6.45E-01
				Sc1	8.33E+00	1.75E-01	9.24E-01	1.80E-01	1.28E+00
				Sc3	1.39E+00	3.91E-02	3.72E-01	1.10E-01	5.21E-01
138261-41-3	Imidacloprid	8.30E-03	Neonicotinoid Insecticide	Sc2	8.43E+00	6.12E-01	8.37E-01	2.80E-01	1.73E+00
				Sc1	1.01E+02	8.86E-01	9.60E-01	5.60E-01	2.41E+00
				Sc3	2.77E+01	3.66E-01	5.23E-01	4.10E-01	1.30E+00
2032-65-7	Methiocarb	2.00E-03	Insecticide/ Herbicide	Sc2	1.25E+01	8.39E-01	9.75E-01	2.80E-01	2.09E+00
				Sc1	4.88E+01	1	1	0.28	2.28
				Sc3	7.00E+00	2.75E-01	6.71E-01	2.80E-01	1.23E-00
19666-30-9	Oxadiazon	8.80E-02	Herbicide	Sc2	2.84E-01	4.29E-03	2.64E-01	0.00E+00	2.68E-01
				Sc1	2.95E+02	8.78E-02	5.38E-01	2.80E-01	9.06E-01
				Sc3	2.84E-01	2.71E-03	2.74E-01	0.00E+00	2.77E-01
111988-49-9	Thiacloprid	1.00E-02	Neonicotinoid Insecticide	Sc2	1.00E+00	4.01E-02	2.93E-01	7.00E-02	4.03E-01
				Sc1	1.18E+01	5.93E-01	7.34E-01	1.80E-01	1.51E+00
				Sc3	1.00E+00	1.54E-02	1.81E-01	4.00E-02	2.37E-01

CAS	Substance	PNEC (µg/L)	Type	Scenario	RQ(p95)	Fspat	Ftemp	Fext	STE score
153719-23-4	Thiamethoxam	4.20E-02	Neonicotinoid Insecticide	Sc2	4.04E-01	7.02E-03	3.89E-01	4.00E-02	4.36E-01
				Sc1	4.52E+00	1.62E-01	5.97E-01	1.10E-01	8.69E-01
				Sc3	3.57E-01	4.19E-03	3.32E-01	4.00E-02	3.76E-01
2303-17-5	Tri-allate	4.10E-01	Herbicide	Sc2	6.10E-02	5.55E-05	0.00E+00	0.00E+00	5.55E-05
				Sc1	3.05E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
				Sc3	6.10E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00

The next figure shows a comparison of STE scores obtained by combined dataset (first WL and last monitoring prioritisation) for scenarios Sc1, Sc2 and Sc3 considering the updated PNECs.



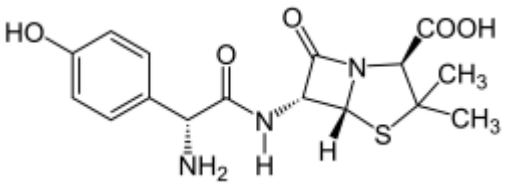
The table below gives per substance for Sc3 information for the site (Fs,site) and country (Fs,country) frequency of exceedances in Fspat, the calculation of Ftemp by all sites (Ftemp_1) and excluding sites with a single measurement that exceeds PNEC (Ftemp_2), the size of the exceedance extent in Fext, the percentage (from the total number of samples) of samples that exceed PNEC and the total amount of samples.

Substance	PNEC (µg/L)	Type	Fs,site	Fs,country	Ftemp_1	Ftemp_2	EXCextent	Exceeding samples (%)	Number of samples (Sc3)
17-alpha-Ethinylestradiol	3.50E-05	Estrogen	3.02E-01	7.14E-01	7.20E-01	5.36E-01	9.83E+00	16.63	469
17-beta-Estradiol	4.00E-04	Estrogen	1.95E-01	4.50E-01	8.58E-01	6.72E-01	4.50E+00	9.78	716
2,6-Di-tert-butyl-4-methylphenol	3.16	Antioxidant	7.75E-03	0.00E+00	7.89E-02	7.89E-02	5.00E-01	0.46	1293
2-Ethylhexyl-4-methoxycinnamate	6	Sunscreen	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.00E-01	0.00	543
Acetamiprid	0.5	Neonicotinoid Insecticide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.31E-02	0.00	7121
Azithromycin	0.019	Antibiotic	3.17E-01	6.50E-01	8.33E-01	7.53E-01	1.53E+01	23.34	1217
Clarithromycin	0.12	Antibiotic	1.20E-01	2.00E-01	3.42E-01	3.35E-01	1.89E+00	5.27	7443
Clothianidin	0.13	Neonicotinoid Insecticide	3.29E-03	4.17E-02	1.88E-01	1.88E-01	1.92E-01	0.29	5952
Diclofenac	0.05	Analgesic	6.06E-01	7.31E-01	5.92E-01	5.70E-01	1.34E+01	44.39	17748
Erythromycin	0.2	Antibiotic	2.50E-02	0.00E+00	2.51E-01	2.18E-01	6.30E-01	0.51	6313
Estrone	0.0036	Estrogen	1.12E-01	3.48E-01	5.19E-01	3.72E-01	5.47E+00	6.09	1314
Imidacloprid	0.0083	Neonicotinoid Insecticide	5.75E-01	6.36E-01	6.01E-01	5.23E-01	5.78E+01	33.38	24745
Methiocarb	0.002	Insecticide/ Herbicide	3.94E-01	7.00E-01	8.49E-01	1.53E-01	1.00E+00	13.56	2781
Oxadiazon	0.088	Herbicide	3.12E-02	8.70E-02	2.74E-01	2.63E-01	6.04E-01	0.94	50148
Thiacloprid	0.01	Neonicotinoid Insecticide	8.87E-02	1.74E-01	2.11E-01	1.81E-01	1.86E+00	2.89	8533
Thiamethoxam	0.042	Neonicotinoid Insecticide	5.03E-02	8.33E-02	3.32E-01	3.00E-01	1.01E+00	1.78	9041
Tri-allate	0.41	Herbicide	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.22E-01	0.00	20725

Annex 9: Factsheets

Amoxicillin (CAS N. 26787-78-0)

Substance identity

EC name	
EC number	
CAS number	26787-78-0
Molecular formula	$C_{16}H_{19}N_3O_5S$
Molecular weight	365.4 g/mol
Structure	
SMILES	

Physico-chemical properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	3430	https://www.drugbank.ca/drugs/DB01060
Log K_{ow}	0.87	Moarefian et al., 2014

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}		
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Amoxicillin has a hydrolysis half-life in water at pH 7 of ca. 20 days.	Braschi, et al., 2013
Bioaccumulation (BCF)		

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	0.006-0.011	Denmark
Uses	Beta-lactam antibiotic	
Spatial usage (by MS)		
	Use in fish farms in 2012-2016.	Denmark
	Widely used in the UK for both human and animal health. Available data note it is one of the most commonly used antibiotics for human health used in the UK. Various products approved for veterinary use on a range of animals including cats, dogs, sheep, pigs, chickens, turkeys, ducks and cattle.	UK
Banned uses		
ERC code		
PEC_{fw} (µg/L)	0.0068	(Besse and Garric, 2008)
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values (µg/l)
In Sc2 (inland whole water) data from only 1 MS (4 sites) with 86 samples are available. No quantified samples. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.01 (Sc2)
Spain	Hospital wastewater, and urban WWTP effluent in Girona (Gros et al., 2013)	0.218-0.258
Europe (90 samples from 18	WWTP effluents	< 0.025

countries)	Loos et al. (2013)	
France	Seine River (Dinh et al., 2011)	0.068
Canada	Wascana Creek, Qu'Appelle River (Waiser et al., 2011)	0.080 (max)
Italy	River Po (Zuccato et al., 2010)	<0.002
Italy	River Arno (Zuccato et al., 2010)	0.006 (mean); 0.010 (max)
UK (Wales)	River Taff and Ely (Kazprzyk-Horden et al., 2008)	0.117 (median); 0.622 (max)
UK (Wales)	River Taff (Kazprzyk-Horden et al., 2007)	<0.010 – 0.245
Italy	WWTP effluents (Castiglioni et al., 2005)	0.015 – 0.120
Italy	Different WWTP effluents (Andreozzi et al., 2004)	0.0018 – 0.120
CZ	No findings in 650 water samples from 52 sites (LOQ: 0.02 - 0.1 µg/l)	< 0.1
UK	Monitored at approximately 80 sites (approx. 1700 samples).	Not detected in any of the samples.

Analytical Methods

Method	**LOQ (µg/l)**	**Description / Reference**
SPE-LC-MS-MS	0.010	(Kazprzyk-Horden et al., 2007)
SPE-LC-MS-MS	0.004	Extraction of 100 ml water; positive ionisation; mass transitions 366 > 349, 114 (Gros et al. (2013)

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Amoxicillin	-	-	-	-

Amoxicillin has a hydrolysis half-life in water at pH 7 of ca. 20 days (Braschi, et al., 2013).

In water, amoxicillin is rapidly degraded by biotic and abiotic factors, yielding different intermediate products; these are suspected of being more resistant to degradation, and potentially more toxic, than the parent compound (Elizalde-Velázquez, 2016).

Amoxicillin may bioaccumulate in fish muscle tissues, with the possibility of the occurrence of these drugs in food, leading to a passive consumption of this antibiotic resulting in undesirable effects on consumer health such as immunoallergic responses. However, the main problem related with the presence of this antimicrobial compounds in fish tissues is the possibility of inducing bacterial resistance genes (Elizalde-Velázquez, 2016).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae			
Pseudokirchneriella subcapitata	72 h Growth inhibition	EC10	>1500000
Pseudokirchneriella subcapitata	7 d Growth inhibition	NOEC	250000
Synechococcus leopolensis	96 h Cell proliferation	NOEC	0.78
Isochrysis galban	96 h Growth inhibition	NOEC	250000
Phaeodactylum tricornutum	96 h Growth inhibition	NOEC	250000
Plants			
Lemna gibba	7 d	EC10	>1000
Invertebrates			

Brachionus calyciflorus	- Average lifespan, net reproductive rate, generational time	LOEC (NOEC)	50 (25)
Brachionus calyciflorus	Gross reproductive rate	NOEC	50
Brachionus calyciflorus	Average lifespan	NOEC	50
Brachionus calyciflorus	Gross reproductive rate, net reproductive rate, rate of population increase	LOEC (NOEC)	50 (25)
Arbacia lixula	72 h Development	EC10	1276000
Parcentrotus lividus	48 h Development	EC10	108000

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	96 h, cell proliferation *Synechococcus leopolensis*	0.78	10	0.078
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	1.28 (Sc2)[a]

[a] RQ is not reliable due to the low quality of MEC value

STE score

n/a (since data scarcity)

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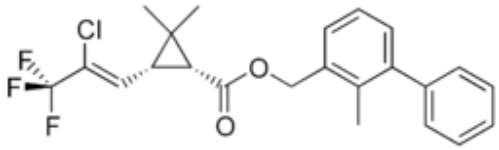
Bifenthrin (CAS N. 82657-04-3)

Substance identity

EC name	
EC number	
CAS number	82657-04-3
Molecular formula	$C_{23}H_{22}ClF_3O_2$
Molecular weight	422.87 g/mol
Structure	 Bifenthrin is a mixture of 2 optical isomers, (Z)-(1R)-cis-acid and (Z)-(1S)-cis-acid (enantiomers)
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	< 0.001	http://npic.orst.edu/factsheets/archive/biftech.html EFSA, 2011
Log K_{ow}	6.0 6.6	https://pubchem.ncbi.nlm.nih.gov/compound/bifenthrin EFSA, 2011

Environmental fate

Endpoint	**Value**	**Source**
Sorption potential K_{oc}	236610	EFSA, 2011
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	EFSA, 2011
Bioaccumulation (BCF)	1703	EFSA, 2011

Pyrethroid insecticides are strongly hydrophobic. As such, the water-soluble fraction of pyrethroids introduced into an aquatic system will be short-lived and quickly reduced. Subsequently, much of the fate and transport of pyrethroids in aquatic systems is

governed by particulate adsorption. Pyrethroid transport within aquatic systems occurs through movement of pyrethroid absorbed fine particulates. Although the half-lives of most pyrethroid insecticides are in the order of days to weeks in the water column, pyrethroids adsorbed to particulates are considerably more persistent, with reported half-lives on sediments of 150 to 200 days. Pyrethroids in stream water are most frequently associated with suspended solids and particulates, with only 0.4% to 1.0% of added pyrethroids present in the freely dissolved phase (Palmquist et al., 2012).

Pyrethroids are most commonly introduced into aquatic systems via runoff from sprayed fields, lawns, parking lots, etc., during rainstorm events, and, to a lesser extent though spray drift (Palmquist et al., 2012).

Due to their high hydrophobicity, pyrethroids readily associate with sediment particles after entering aquatic systems and are one of the major threats to benthic invertebrates in urban waterways (Chen et al., 2015; Ding et al., 2010; Kuivila et al., 2012).

Their high hydrophobicity, along with pseudo-persistence due to continuous input, indicates that pyrethroids will accumulate in sediment, pose long-term exposure concerns to benthic invertebrates and ultimately cause significant risk to benthic communities and aquatic ecosystems. The current study has provided evidence that pyrethroids are not only commonly detected in the aquatic environment, but also can cause toxic effects to benthic invertebrates, and calls for better development of accurate sediment quality criteria and effective ecological risk assessment methods for this emerging class of insecticides (Li et al., 2017).

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year		
Uses	Bifenthrin is approved as PPP in the EU (12 MS: AT, BE, CY, DE, ES, FI, FR, GB, IT, LU, NL, PO). The approval is in progress for AT and CZ	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1026 https://echa.europa.eu/it/information-on-chemicals/pic/import-notifications?p_p_id=importnotifications_WAR_echapicportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_importnotifications_WAR_echapicportlet_highlightedsearch=true&_importnotifications_WAR_echapicportlet_highlightedname=Bifenthrin&_importnotifications_WAR_echapicportlet_highlightedcasnumber=82657-04-3
	Only uses as insecticide may be authorised.	http://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:32012R0582&from=EN
Spatial usage (by MS)		
	Northern Ireland: used in agriculture	UK

Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 3 MS (1132 sites) with 7572 samples are available. Only 0.03% quantified samples. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.025 µg/l (Sc2)
UK	Monitored at approx. 500 sites as part of national catchment sensitive farming (CSF) & watch list programmes and WFD national surveillance programme.	Not detected in any samples.

California's Stream Pollution Trends program assesses long-term water quality trends, using 100 base-of-the-watershed sampling sites. A significant increasing trend for pyrethroid pesticide concentrations in sediment samples was observed throughout the state, likely associated with an increasing trend of pyrethroid use in urban watersheds. There were no significant increasing or decreasing trends for pyrethroids in agriculturally dominated or open space watersheds. Bifenthrin was the most commonly detected pyrethroid and was measured in 69% of the samples (n=410) over the five year study. The remaining pyrethroids, including cyfluthrin, cyhalothrin, cypermethrin, deltamethrin, esfenvalerate/fenvalerate, fenpropathrin, and permethrin, were detected in 19% to 39% of the samples (Siegler et al., 2015).

Currently used agricultural pesticides were monitored in sediments in California's Central Valley. The pyrethroid bifenthrin in particular, as well as lambda-cyhalothrin, cypermethrin, esfenvalerate, permethrin, and the organophosphate chlorpyrifos, were primarily responsible for the observed sediment toxicity in these agricultural sediments (Weston et al., 2013).

Corcellas et al. (2015) described for the first time pyrethroid pesticide bioaccumulation in edible river fish collected in 4 different Iberian rivers, and conclude that pyrethroid levels are safe for human consumption taken into account the current regulations.

Pyrethroids have mainly been analysed in sediment (Amweg et al., 2005; Delgado-Moreno et al., 2011; Hintzen et al., 2009; Li et al., 2017; Siegler et al., 2015; Weston et al., 2011; 2013), and only a few times in water (Delgado-Moreno et al., 2011; Feo et al., 2010; Weston and Lydy, 2010), or biota (Brodeur et al., 2017; Corcellas et al., 2015).

Tang et al. (2018) give a world-wide overview on pyrethroid pesticide residues in the global environment.

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
GC-MS	0.001	In surface water (EFSA, 2008 and EFSA, 2011).
GC-NCI-MS	0.00004	Extraction by ultrasound-assisted emulsification-extraction of a water-immiscible solvent (chloroform) in 20 mL water (Feo et al., 2010).
GC-ECD/MS	0.00006–0.00098 (LOD)	SPE (Zheng et al., 2016).
n.a.	0.005	Finland

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Bifenthrin	P, B and T		ED	

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)

Invertebrates			
Daphnia magna	21 d	NOEC	0.00095
Daphnia magna	21 d	NOEC	0.0013
Corbicula	21 d	NOEC	2.58
Mysidopsis bahia	28 d	NOEC	0.0012
Chironomus riparius	28 d	NOEC	0.32
Fish			
Pimephales promelas	21 d	NOEC	1.86
Pimephales promelas	368 d	NOEC	0.04

Mammalian toxicology data

PNEC derivation

PNEC	**Endpoint (µg/l)**	**Endpoint value (µg/l)**	**AF**	**PNEC value (µg/l)**
$PNEC_{fw}$	NOEC, 21 d (*Daphnia magna*)	0.00095	50	0.00002
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	**Value**
RQ_{fw} (for MEC(P(95)) and	1250 (Sc2)

PNEC=0.00002 µg/l)	
RQ_{fw} (for PEC=0.054 µg/l and PNEC= 0.00002 µg/l)	2700
RQ_{fw} (for PEC=0.0049 µg/l and PNEC= 0.00002 µg/l)	245

Note: PEC values are taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based strategy for the prioritisation exercise under the Water Framework Directive,* https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

3 (Sc2)

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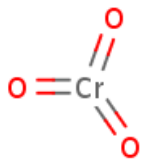
Chromium trioxide and other Cr(VI) compounds (CAS N. 1333-82-0; 18540-29-9)

Substance identity

EC name	
EC number	
CAS number	1333-82-0; 18540-29-9 (Chromium(VI))
Molecular formula	CrO3; Cr(VI)
Molecular weight	99.99; Cr(VI): 51.9
Structure	
SMILES	[Cr](=O)(=O)=O

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)	Not available (inorganic ionic compound)	EU-RAR, 2005[1]
Water solubility (mg/L)	1667 mg/L	EU-RAR, 2005[1]
Log K_{ow}	Not available (inorganic ionic compound)	EU-RAR, 2005[1]

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	Not available	EU-RAR, 2005[1]
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)	1000	EU-RAR, 2005[1]
Biodegradability	N.a.	EU-RAR, 2005[1]
Bioaccumulation (BCF)	2.8	EU-RAR, 2005[1]

Chromium is a relatively common element and occurs in the earth's crust at an average concentration of 200 mg/kg. In soils one finds in general contents of 10 to 90 mg/kg.

Trivalent chromium is an essential trace element for humans and animals. Hexavalent chromium compounds cause allergic and asthmatic reactions and are considered carcinogenic.

Chromium occurs in waters in trivalent and hexavalent form. Under aerobic conditions chromium (VI) is stable. Under anaerobic conditions, it is reduced to Chromium (III). Under oxidizing conditions a transformation from chromium (III) to chromium (VI) is also possible. The distribution between chromium (III) and chromium (VI) of the total chromium concentration in flowing waters is not constant, chromium (VI) has a share of 30-70%.

Due to the formation of poorly soluble chromium (III) compounds and adsorption of chromium in suspended solids, a large part of the chromium is particulate bound.

There is a wide range of background values ("ambient background concentrations") within Europe. For the dissolved concentration of chromium in uncontaminated waters, values of <0.1 µg/L to 0.5 µg/L are given. The FOREGS study gives for European waters for >0.45 µm filtered concentration a median value (n = 806) of 0.38 µg/L.

(Internationale Kommission zum Schutz des Rheins, 2009).

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year	114 (2010) in CZ	CZ
Uses	Manufacture of substances and of preparations, formulation of preparations and materials, industrial use resulting in inclusion into or onto a matrix, use as laboratory reagent. Chromium trioxide meets the criteria for inclusion in Annex XIV to Regulation (EC) N. 1906/2006[3]. In 2015 the latest application date were expected for chromium trioxide is 21 March 2016, and the sunset date is 21 September 2017[4], but exemptions have been granted for certain uses.	ECHA, 2013[2] Regulation (EC) N. 1906/2006[3] COMMISSION REGULATION (EU) No 348/2013[4]
	Electroplating.	CZ
	Main source is leather tanning industry and other industries using chromium.	DK
Spatial usage (by MS)	Not known	-
Banned uses	Cement and cement-containing mixtures shall not be placed on the market, or used, if they contain, when hydrated, more than 2 mg/kg (0,0002%) soluble chromium VI of the total dry weight of the cement. Leather articles coming into contact with the skin shall not be placed on the market where	ECHA, List of substances restricted under REACH[5]

	they contain chromium VI in concentrations equal to or greater than 3 mg/kg (0,0003 % by weight) of the total dry weight of the leather. Articles containing leather parts coming into contact with the skin shall not be placed on the market where any of those leather parts contains chromium VI in concentrations equal to or greater than 3 mg/kg (0,0003 % by weight) of the total dry weight of that leather part.	
ERC code	-	-
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)	0.98 (N.R.)	Calculation based on Equation L (Section 3.4.3)

N.R. Not required based on BCF value not reaching the trigger value required for biota assessment

Measured Environmental Concentrations

Chromium is analysed in most countries as total chromium (VI+III). In the prioritisation exercise 2014, Cr(VI) data were only available for non-filtered water samples (whole water fraction) from 4 countries.

In 2018, one MS (England) submitted Cr(VI) data for dissolved water samples, and 9 MS total chromium (VI+III) data.

The use of monitored concentrations for chromium total in dissolved fraction, and the use of monitored concentration for Cr(VI) in whole water, below, gives an overestimation of the risk posed by Chromium VI in dissolved fraction.

MS	Source of monitoring data	MEC values
Cr(VI) in Sc3 (inland whole water) in 4 countries	415 samples (93% quantified) (Dataset of monitoring prioritisation 2014)	6 µg/l (P95)
Cr(total) in Sc3 (inland dissolved fraction) in 24 countries	134937 samples (22.8% quantified) (Dataset of monitoring prioritisation 2014 + data submitted in 2018; years 2010-2018)	1.0 µg/l (P95) 0.25 µg/l (median)
Cr(total) in Sc3 (coastal and transitional water) in 6 countries	370 samples (23% quantified) (Dataset of monitoring prioritisation 2014)	0.7 µg/l (P95) 0.5 µg/l (median)

Cr(total) in CZ	Waste water; measured in industrial waste water; not in surface water. Year 2015.	0.02-497 µg/l
Cr(VI) in England (probably dissolved phase)	Approx. 170 sites monitored quarterly in water body's deemed at risk from Cr(VI) via permitted discharges.	Results mostly show below LOD however 1 site exceeds AA EQS, and 2 others record values above this limit.
Cr(VI) in dissolved water phase in England	Number of samples: 5724; quantified samples (> LOQ): 1716; LOQ (µg/L): 0.1-0.6. Number of samples in Sc3: 5724.	0.05 µg/l (median) 0.30 µg/l (P95)

Analytical Methods

Method	**LOQ (µg/l)**	**Description / Reference**
EPA method 218.7 (2011)	0.0044 to 0.015 (LOD)	Samples are preserved with a combined buffer/dechlorinating reagent which complexes free chlorine and increases the pH to a value greater than eight. A measured volume (usually 1 mL) of the sample is introduced into an ion chromatograph. CrO_4^{2-} is separated from other matrix components on an anion exchange column. CrO_4^{2-} is derivatized with 1,5-diphenylcarbazide in a post-column reactor and is detected spectrophotometrically at a wavelength of 530 nm. Cr(VI) is qualitatively identified via retention time, and the concentration of CrO_4^{2-} in the sample is calculated using the integrated peak area and the external standard technique. Results are reported in units of µg/L of Cr(VI) (EPA method 218.7; 2011).
Ion chromatography	LOD: 0.050 LOQ: 0.16	Cr(VI) determination in water samples with ion chromatography followed by post-column derivatization of the Cr(VI) with diphenylcarbazide and detection of the colored complex at 530 nm. (Mamais et al., 2016).
LC-ICP-MS	0.001 to 0.01 (LOD)	Perkin Elmer Application note; Vonderheide et al, 2004.
ISO method 23913:2006 Flow analysis (FIA	2-200 (LOD)	ISO 23913:2006 specifies flow injection analysis (FIA) and continuous flow analysis (CFA) methods for the determination of chromium(VI) in various types of water. The method applies to

and CFA) and spectrometric detection		the following mass concentration ranges: for FIA (20 to 200 micrograms per litre and 200 to 2 000 micrograms per litre for surface water, leachates and waste water) and for CFA (2 to 20 micrograms per litre and 20 to 200 micrograms per litre for drinking water, ground water, surface water, leachates and waste water). The range of application may be changed by varying the operating conditions. Seawater may be analysed by these methods with changes in sensitivity and after adaptation of the reagent and calibration solutions to the salinity of the samples.
Ion chromatography	1	Ionic chromatography to separate Cr6+ and interfering compounds. Measure by spectrometry (540nm) after derivation post column by 1.5-diphenylcarbazide solution (Belgium-Wallonia).

Hazard properties

Substance	Persistent(P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)
Chromium (VI)	P and T	M and R	Not investigated

The evidence clearly indicates that highly water-soluble Cr(VI) compounds can produce significant mutagenic activity in vitro and in vivo[1]. The Cr (VI) compounds under consideration are therefore regarded as in vivo somatic cell mutagens[1]. In addition, toxicokinetic and dominant lethal data suggest that water-soluble Cr (VI) has the potential to be an in vivo germ cell mutagen[1]. Chrome plating workers exposed to chromium (VI) trioxide in aqueous solution have shown a clear excess in mortality from lung cancer[1]. Therefore chromium (VI) trioxide should be regarded as a human carcinogen[1]. Adverse effects on fertility have been found in studies in mice following repeated oral exposure[1]. In addition, adverse effects on the testes have been seen following repeated oral exposure in the rat (EU-RAR, 2005[1]). The substance is not readily biodegradable (P). It shows a low potential to bioaccumulate in aquatic organism[1].

Hazard assessment

Ecotoxicology data

Chromium (VI)

The PNEC previously used for chromium (VI) in the 2014 prioritisation report has been updated by JRC after a literature search and the evaluation of new chronic toxicity data. The assessment performed in the European Risk Assessment Report (EU 2005), by the Environment Agency in 2007 (UK EA 2007) and in the UBA Dossier 2015 have been taken into consideration, with the inclusion of additional chronic data assessed to be adequate and relevant. On this basis, the JRC has derived a new PNEC of 2.06 µg/L for chromium (VI).

In addition to the previous chronic quality standard derivation (EU 2005), 31 freshwater and 2 marine water chronic toxicity values have been found from 17 studies published after 2005. A literature evaluation of these studies has been performed by using the LET tool in-house developed by the JRC, and based on the work of Kase et al. (2015), and three of them were deemed to be not reliable. Freshwater and marine water datasets have been treated separately, in accordance with the EQS Technical Guidance Document (EC 2011).

An overall dataset of 73 freshwater chronic toxicity values are available for 35 species of 8 different taxonomic groups, i.e. 7 algae species, 2 cnidarian species, 5 crustaceans, 11 fish species, 4 higher aquatic plants, 2 insects, 2 molluscs, and 2 amphibians.

After selecting the most sensitive geometric mean endpoints per species, a probabilistic approach has been undertaken with 35 freshwater chronic data points, giving an HC5 value of 0.006 mg/L. An AF of 3 has been applied to the HC5 value giving a chronic freshwater QS of 2.06 µg/L.

Regarding the marine water chronic toxicity dataset, only a deterministic approach could be applied, since data are available for 15 species of 5 taxonomic groups. The lowest value has been observed for the polychaete worm *Nereis arenaceodentata* with a 2-week NOEC of 0.006 mg/L. In accordance with the EQS Technical Guidance Document (EC 2011), an AF of 10 has been applied, giving a chronic marine water QS of 0.6 µg/L.

CHRONIC EFFECTS			**Master Reference**
Algae (mg/L)	**Freshwater**	*Chlorella pyrenoidosa* / 96 h / Biomass NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Meisch and Schmitt-Beckmann 1979
		Chlorella sp. (wild) / 96 h / Biomass NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Meisch and Schmitt-Beckmann 1979
		Chlorella vulgaris / 96 h / Growth inhibition LOEC : 0.0026 mg/L	Ouyang et al. 2012 (Klimisch 2; supporting information)*
		Chlorella vulgaris / 96 h / Percentage of inhibition NOEC : 2.6 mg/L	Qian et al. 2013 (Klimisch 2)*
		Microcystis aeruginosa / 8 d / Biomass NOEC : 0.002 mg/L	EU, 2005; UK EA, 2007; Bringmann and Kühn 1978 (Klimisch 3)
		Microcystis aeruginosa / 7 d / Chlorophyll EC_{50} : 0.211 mg/L	ECOTOX DB; UK EA, 2007; Halling-Sorensen 2000
		Microcystis aeruginosa / 96 h / Growth rate NOEC : 0.35 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Scenedesmus pannonicus / 96 h / Biomass NOEC : 0.11 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Scenedesmus subspicatus / 72 h / Biomass EC_{10} : 0.032 mg/L	EU, 2005; UK EA, 2007; Kühn and Pattard 1990
		Scenedesmus subspicatus / 72 h / Growth EC_{10} : 0.64 mg/L	EU, 2005; Kühn and Pattard 1990
		Pseudokirchneriella subcapitata / 72 h / Growth rate EC_{10} : 0.11 mg/L	EU, 2005; UK EA, 2007; Nyholm 1991
		Pseudokirchneriella subcapitata / 72 h / Growth rate	EU, 2005; UK EA, 2007; Christensen and Nyholm 1984

CHRONIC EFFECTS			Master Reference
		EC_{10} : 0.01 mg/L	
	Marine water	*Gracilaria tenuistipitata* / 96 h / Population growth NOEC : 0.04 mg/L	ECOTOX DB; UK EA, 2007; Haglund et al. 1996
		Gracilaria tenuistipitata / 96 h / Population growth NOEC : 0.26 mg/L	ECOTOX DB; UK EA, 2007; Haglund et al. 1996
		Thalassiosira pesudonana / 15 d / Growth inhibition NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Frey et al. 1983
Higher aquatic plants (mg/L)	**Freshwater**	*Lemna gibba* / 8 d / Growth biomass NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Staves and Knaus 1985
		Lemna minor / 7 d / Growth NOEC : 0.11 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Lemna minor / 7 d / Growth rate dry weight EC_{10} : 0.047 mg/L	Naumann et al. 2007 (Klimisch 2)*
		Lemna minor / 7 d / Growth rate fresh weight EC_{10} : 0.036 mg/L	Naumann et al. 2007 (Klimisch 2)*
		Lemna minor / 7 d / Growth rate frond number EC_{10} : 0.047 mg/L	Naumann et al. 2007 (Klimisch 2)*
		Spirodela polyrhiza / 8 d / Growth NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Staves and Knaus 1985
		Spirodela punctata / 8 d / Growth NOEC : 0.5 mg/L	EU, 2005; UK EA, 2007; Staves and Knaus 1985
Invertebrates (mg/L)	**Freshwater**	*Hydra littoralis* / 11 d / Reproduction Threshold : 0.035 mg/L	EU, 2005; UK EA, 2007; Dannerberg 1984
		Hydra oligactis / 21 d / Growth rate NOEC : 1.1 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Ceriodaphnia dubia / 7 d / Reproductiom NOEC : 0.015 mg/L	Baral et al. 2016 (Klimisch 3)*
		Ceriodaphnia dubia / 7 d / Reproduction NOEC : 0.0045 mg/L	Rodgher and Espindola 2008 (Klimisch 2)*
		Ceriodaphnia dubia / 7 d / Reproduction NOEC : 0.0047 mg/L	EU, 2005; UK EA, 2007; De Graeve et al. 1992
		Ceriodaphnia dubia / 7 d / Reproduction IC_{50} : 0.013 mg/L	EU, 2005; UK EA, 2007; De Graeve et al. 1994
		Ceriodaphnia dubia / 7 d / Survival NOEC : 0.0084 mg/L	EU, 2005; UK EA, 2007; De Graeve et al. 1993
		Daphnia carinata / 14 d / Reproduction NOEC : 0.05 mg/L	EU, 2005; UK EA, 2007; Hickey 1989
		Daphnia magna / 21 d / Growth NOEC : 0.06 mg/L	EU, 2005; UK EA, 2007; Van Leeuwen et al. 1987
		Daphnia magna / 63 d / Growth NOEC : 0.0035 mg/L	UK EA, 2007; Gorbi et al. 2002
		Daphnia magna / 21 d / Mortality NOEC : 0.018 mg/L	EU, 2005; UK EA, 2007; Kühn et al. 1989
		Daphnia magna / 21 d / Mortality NOEC : 0.035 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983

CHRONIC EFFECTS			Master Reference
		Daphnia magna / 21 d / Reproduction NOEC : 0.018 mg/L	EU, 2005; UK EA, 2007; Kühn et al. 1989
		Daphnia magna / 21 d / Reproduction NOEC : 0.035 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Daphnia magna / 14 d / Reproduction NOEC : 0.025 mg/L	EU, 2005; UK EA, 2007; Hickey 1989
		Daphnia magna / 63 d / Reproduction NOEC : 0.0035 mg/L	UK EA, 2007; Gorbi et al. 2002
		Daphnia magna / 14 d / Reproduction NOEC : 0.0005 mg/L	EU, 2005; UK EA, 2007; Elnabarawy et al. 1987
		Daphnia magna / 21 d / Survival NOEC : 0.2 mg/L	EU, 2005; Van Leeuwen et al. 1987
		Daphnia magna / 63 d / Survival NOEC : 0.0035 mg/L	UK EA, 2007; Gorbi et al. 2002
		Daphnia magna / 14 d / Survival NOEC : 0.015 mg/L	EU, 2005; UK EA, 2007; Elnabarawy et al. 1986
		Daphnia magna / 28 d / Survival/reproduction NOEC : <0.010 mg/L	EU, 2005; UK EA, 2007; Trabalka and Gehrs 1977
		Daphnia magna / 21 d / Yield NOEC : 0.35 mg/L	EU, 2005; Van Leeuwen et al. 1987
		Hyalella azteca / 28 d / Biomass NOEC : 0.0092 mg/L	Wang et al. 2017 (Klimisch 2)*
		Hyalella azteca / 28 d / Biomass NOEC : 0.042 mg/L	
		Hyalella azteca / 28 d / Dry weight NOEC : 0.019 mg/L	
		Hyalella azteca / 28 d / Dry weight NOEC : 0.021 mg/L	
		Hyalella azteca / 28 d / Survival NOEC : 0.036 mg/L	
		Hyalella azteca / 28 d / Survival / NOEC : 0.021 mg/L	
		Pseudosida ramosa / 21 d / Total numbe of eggs and live neaonates NOEC : 0.003 mg/L	Freitas and Rocha 2014 (Klimisch 2)*
		Lampsilis siliquoidea / 28 d / Biomass NOEC : 0.019 mg/L	Wang et al. 2017 (Klimisch 2)*
		Lampsilis siliquoidea / 28 d / Biomass NOEC : 0.01 mg/L	
		Lampsilis siliquoidea / 28 d / Dry weight NOEC : 0.019 mg/L	
		Lampsilis siliquoidea / 28 d / Dry weight NOEC : 0.01 mg/L	
		Lampsilis siliquoidea / 28 d / Survival NOEC : 0.019 mg/L	
		Lampsilis siliquoidea / 28 d / Survival NOEC : 0.01 mg/L	
		Lymnaea stagnalis / 7 d / Hatchability NOEC : 0.35 mg/L	EU, 2005; Slooff and Canton 1983
		Lymnaea stagnalis / 40 d / Mortality NOEC : 3.5 mg/L	EU, 2005; Slooff and Canton 1983

CHRONIC EFFECTS			Master Reference
		Lymnaea stagnalis / 40 d / Reproduction budles NOEC : 0.11 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Culex pipiens / 25 d / Survival/growth 1st instar NOEC : 1.1 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Culex quinquefasciatus / 10 d / Relative growth inhibition NOEC : 0.1 mg/L	Sorensen et al. 2006 (Klimisch 2)*
	Ground water	Budderoo cyclopoid / 28 d / Mortality EC_{10} : 0.08 mg/L	Hose et al. 2016 (Klimisch 2, supporting information)*
		Somersby cyclopoid / 28 d / Mortality EC_{10} : 0.02 mg/L	Hose et al. 2016 (Klimisch 2, supporting information)*
		Somersby harpacticoid / 28 d / Mortality EC_{10} : 0.002 mg/L	Hose et al. 2016 (Klimisch 2, supporting information)*
	Marine water	*Acartia tonsa* / 5 d / Development NOEC : 1 mg/L	ECOTOX DB; UK EA, 2007; Andersen et al. 2001
		Americamysis bahia / 7 d / Growth NOEC : 0.6 mg/L	ECOTOX DB; UK EA, 2007; Jop 1989
		Americamysis bahia / 7 d / Reproduction NOEC : 0.32 mg/L	ECOTOX DB; UK EA, 2007; Goodfellow and Rue 1989
		Cyprinodon variagates / 7 d / Growth larvae NOEC : 3.2 mg/L	ECOTOX DB; UK EA, 2007; McCulloch and Rue 1989
		Cyprinodon variagates / 7 d / Growth larvae NOEC : 2.5 mg/L	ECOTOX DB; UK EA, 2007; Jop 1989
		Mysidopsis bahia / 38 d / Reproduction brood size NOEC : 0.088 mg/L	EU, 2005; UK EA, 2007; Lussier et al. 1985
		Neomysis integer / 14 d / Mortality NOEC : 0.156 mg/L	EU, 2005; UK EA, 2007; Van der Meer et al. 1988
		Oncorhynchus kisutch / 11 d / Mortality NOEC : 17.8 mg/L	ECOTOX DB; UK EA, 2007; Holland et al. 1960
		Palaemon elegans / 38 d / Mortality NOEC : 1.56 mg/L	EU, 2005; UK EA, 2007; Van der Meer et al. 1988
		Petrolisthes laevigatus / 7 d / Mortality NOEC : 20 mg/L	Urrutia et al. 2008 (Klimisch 2)*
		Praunus flexuosus / 23 d / Mortality NOEC : 1 mg/L	EU, 2005; UK EA, 2007; Van der Meer et al. 1988
		Rhithropanopeus harrisii / 19 d / Survival hatch 1st crab NOEC : 0.36 mg/L	EU, 2005; UK EA, 2007; Bookhout et al. 1984
		Rhithropanopeus harrisii / 19 d / Survival to 1st crab stage NOEC : 0.36 mg/L	EU, 2005; UK EA, 2007; Bookhout et al. 1984
		Tisbe battagliai / 8 d / Reproduction /NOEC : 0.32 mg/L	ECOTOX DB; UK EA, 2007; Hutchinson et al. 1994
		Nereis arenaceodentata / 14 d / Mortality NOEC : 0.006 mg/L	EU, 2005; UK EA, 2007; Mearns et al. 1976
		Nereis arenaceodentata / 2 generation / Reproduction F1 generation NOEC : 0.017 mg/L	EU, 2005; UK EA, 2007; Oshida and Word 1982

CHRONIC EFFECTS			Master Reference
		Nereis arenaceodentata / 2 generation / Reproduction reduction in no. Of progeny 2nd generation NOEC : 0.0125 mg/L	EU, 2005; UK EA, 2007; Oshida et al. 1981
Fish (mg/L)	**Freshwater**	*Catostomus commersoni* / 60 d / Growth eggs/fry NOEC : 0.29 mg/L	EU, 2005; UK EA, 2007; Sauter et al. 1976
		Channa punctatus / 60 d / Body weight gain NOEC : 2 mg/L	Mishra and Mohanty 2009 (Klimisch 2)*
		Channa punctatus / 31 d / Growth and development of ovary LOEC : 4 mg/L	Mishra and Mohanty 2008 (Klimisch 3)*
		Esox lucius / 20 d / Mortality eggs/fry NOEC : 0.538 mg/L	EU, 2005; UK EA, 2007; Sauter et al. 1976
		Icatalurus punctatus / 30 d / Growth eggs/fry NOEC : 0.15 mg/L	EU, 2005; UK EA, 2007; Sauter et al. 1976
		Odontesthes bonariensis / 16 d / Growth NOEC : 0.5 mg/L	Carriquiriborde and Ronco 2007 (Klimisch 2)*
		Oncorhynchus mykiss / 8 mo / Growth alevin-juvenile NOEC : 0.1 mg/L	EU, 2005; UK EA, 2007; Benoit 1976
		Oncorhynchus mykiss / 60 d / Growth eggs/fry NOEC : 0.051 mg/L	EU, 2005; UK EA, 2007; Sauter et al. 1976
		Oncorhynchus mykiss / 244 d / Mortality eyed eggs NOEC : 0.02 mg/L	EU, 2005; UK EA, 2007; Van Der Putte et al. 1982
		Oncorhyncus tshawytscha / 7 d / Fertilization NOEC (highest value tested) : 0.266 mg/L	Farag et al. 2006 (Klimisch 3)*
		Oryzias latipes / 40 d / Mortality embryo larvae NOEC : 3.5 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Pimephales promelas / 60 d / Growth egg/larvae NOEC : 1 mg/L	EU, 2005; UK EA, 2007; Pickering 1980
		Pimephales promelas / 30 d / Growth larvae NOEC : 0.05 mg/L	EU, 2005; UK EA, 2007; Broderius and Smith 1979
		Pimephales promelas / 7 d / Growth larvae NOEC : 1.1 mg/L	EU, 2005; UK EA, 2007; De Graeve et al. 1993
		Pimephales promelas / 412 d / Growth larval NOEC : 3.95 mg/L	EU, 2005; UK EA, 2007; Pickering 1980
		Pimephales promelas / 60 d / Survival 4-week juvenile NOEC : 1 mg/L	EU, 2005; UK EA, 2007; Pickering 1980
		Poecilia reticulata / 28 d / Mortality 3-4 weeks NOEC : 3.5 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983
		Salvelinus fontinalis / 8 mo / Growth NOEC : 0.01 mg/L	EU, 2005; UK EA, 2007; Benoit 1976
		Salvelinus namaycush / 60 d /	EU, 2005; UK EA, 2007; Sauter

CHRONIC EFFECTS			Master Reference
		Growth eggs/fry NOEC : 0.105 mg/L	et al. 1976
	Marine water	*Fundulus heteroclitus* / 30 d / Weight NOEC : 1.5 mg/L	Roling et al. 2006 (Klimisch 1)*
Other organisms: Amphibians (mg/L)	**Freshwater**	*Duttaphrynus melanostictus* / 21 d / Mortality LC_{50} : 1 mg/L	Fernando et al. 2016 (Klimisch 2, supporting information)
		Hypsiboas pulchellis / 280 h / Embryo growth inhibition NOEC : 1 mg/L	Natale et al. 2006 (Klimisch 2)*
		Hypsiboas pulchellis / 280 h / Tadpoles growth inhibition NOEC : 3 mg/L	Natale et al. 2006 (Klimisch 2)*
		Xenopus laevis / 100 d / Mortality tadpole NOEC : 0.35 mg/L	EU, 2005; UK EA, 2007; Slooff and Canton 1983

* The reliability of the study was evaluated by using the LET tool in-house developed by the JRC, and based on the work of Kase et al. (2015)

Chromium (III)

In addition a new PNEC of 1.8 µg/L has been derived by JRC for chromium (III) after a literature search and the evaluation of new chronic ecotoxicological data.

In addition to the chronic toxicity values reported in the European Assessment report of 2005 (EU 2005), four toxicological data have been retrieved (2 from the ECHA's dissemination website, and 2 from recent publications), giving a final dataset of 9 freshwater and 2 marine water chronic toxicity values.

The available dataset could not enable the derivation of an SSD curve, since only data from 7 species of three taxonomic groups have been found. Therefore, the deterministic approach has been carried out in the present assessment.

The 30-day time-to-hatch NOEC 0.018 mg/L for the fish *Danio rerio* (Study report 1990, ECHA DB 2018b) has been determined to be the lowest chronic freshwater value in the new dataset. Because data are available from each trophic level of the base set, an AF of 10 has been applied (EC 2011), giving a QS of 1.8 µg/L.

The only value available for the marine water is the 7-day mortality NOEC 40 mg/L of the crustacean *Petrolisthes laevigatus* (Urrutia et al. 2008). Based on these data, it has been yet deemed to be insufficient to derive QS for marine water bodies.

Species	Taxonomic group	Duration	Effect measured	Endpoint	Effect concentration (mg/L)	Reference
Freshwater						
Chlorella pyrenoidosa	Algae	5 d	Cell number	NOEC	0.1	EU 2005 ; Meisch and Schmitt-Beckmann 1979
Scenedesmus subspicatus	Algae	72 h	Growth rate	NOEC	0.004	ECHA dissemination website 2018a

Species	Taxonomic group	Duration	Effect measured	Endpoint	Effect concentration (mg/L)	Reference
						; Study report 2010 (supporting information, value not related to dissolved Cr form)
Ceriodaphnia dubia	Crustaceans	7 d	Reproductiom	NOEC	1.253	Baral et al. 2016 (Klimisch 3)*
Daphnia magna	Crustaceans	--	lifecycle	NOEC	0.047	EU 2005 ; Chapman et al. 1985 (unpublished)
Daphnia magna	Crustaceans	--	lifecycle	NOEC	0.129	EU 2005 ; Chapman et al. 1985 (unpublished)
Daphnia magna	Crustaceans	21 d	Reproduction	NOEC	3.4	EU 2005 ; Kuhn et al. 1989; Dose 1993
Danio rerio	**Fish**	**30 d**	**Time to hatch**	**NOEC**	**0.018**	**ECHA dissemination website 2018b; Study report 1990**
Oncorhynchus mykiss	Fish	72 d	ELS	NOEC	0.05	EU 2005 ; Stevens and Chapman 1984
Pimephales promelas	Fish	5 d	lifecycle	NOEC	0.75	EU 2005 ; Pickering unpublished
Marine water						
Neanthes arenaceodentata	Annelid	--	--	NOEC	>50.1	EU 2005 ; Oshida et al. 1976
Petrolisthes laevigatus	Crustaceans	7 d	Mortality	NOEC	40	Urrutia et al. 2008 (Klimisch 2)

* The reliability of the study was evaluated by using the LET tool in-house developed by the JRC, and based on the work of Kase et al. (2015)

PNEC derivation (Cr(VI))

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	$HC_{5\text{-}50\%}$	6.0	3 (SSD)	2.06

$PNEC_{t+cw}$	NOEC (*Nereis arenaceodentata* / 2-week)	6.0	10	0.6

PNEC derivation (Cr(III))

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	NOEC (*Danio rerio* / 30d)	18	10	1.8

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (CrVI, dissolved) (for MEC(P(95) data from England and PNEC=2.06 µg/L)	0.12 (Sc3)
RQ_{fw} (Cr(total), dissolved) (for MEC(P(95) data from 24 countries for time period 2010-2018, and PNEC=1.8 µg/L)	0.56 (Sc3)
RQ_{c+tw} (Cr(total), dissolved) (for MEC(P(95) data from 6 countries and PNEC=0.6 µg/L)	1.17 (Sc3)
RQ_{fw} (PEC/PNEC)	102.94[a]

[a] PEC has been derived for the 1st WL and it doesn't consider the restricted use. (Carvalho, et al., WL report 2015)

STE score (Sc3)

1.099 (PNEC=2.06 µg/L) (Cr(VI) inland whole water; data from 4 countries).

0.203 (PNEC=1.8 µg/L) (Cr(total) inland dissolved phase; data from 24 countries).

0.564 (PNEC=0.6 µg/L) (Cr(total) coastal and transitional dissolved phase; data from 6 countries).

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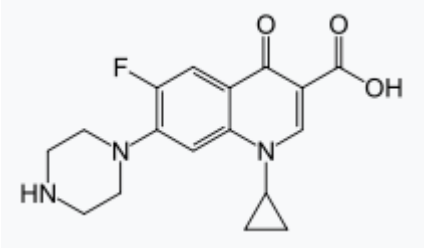
Ciprofloxacin (CAS N. 85721-33-1)

Substance identity

EC name	
EC number	
CAS number	85721-33-1
Molecular formula	$C_{17}H_{18}FN_3O_3$
Molecular weight	331.3 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	30	https://pubchem.ncbi.nlm.nih.gov/compound/ciprofloxacin#section=Top
Log K_{ow}	0.28	https://pubchem.ncbi.nlm.nih.gov/compound/ciprofloxacin#section=Top

Environmental fate

Although several studies have reported the presence of ciprofloxacin in wastewater effluent and surface water (see table below), the half-life of ciprofloxacin in surface water is expected to be short due to rapid bio- (Amorim et al., 2013) and photodegradation (Cardoza et al., 2005; Lam et al., 2003; Sturini et al., 2012) with reported half-lives in surface water between 10 days (Van Doorslaer et al., 2014) and 2 h (Lam et al., 2003; Cardoza et al., 2005). Ciprofloxacin also tends to adsorb to particles with a log K_{oc} value of 4.8 l/kg for soil (Nowara et al., 1997) and log K_{oc} values of 4.3–4.9 l/kg (dependent on pH) for fine particulate matter (Cardoza et al., 2005). In conclusion, both adsorption and photodegradation strongly influence ciprofloxacin fate in aquatic systems, although the dominant mechanism appears to depend upon the ambient SPM level (Cardoza et al., 2005).

Endpoint	Value	Source

Sorption potential log K_{oc}	Possible FQ removal mechanisms during wastewater treatment are biodegradation and sorption on activated sludge. 4.3–4.9 l/kg (SPM) 4.8 l/kg (soil)	Van Doorslaer et al., 2014; Cardoza et al., 2005 Nowara et al., 1997
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Half-life time in surface water: 2 h - 10.6 days	Andreozzi et al., 2003; Cardoza et al., 2005; Van Doorslaer et al., 2014.
Bioaccumulation (BCF)		

Note that ciprofloxacin is a degradation product of enrofloxacin (Babic et al., 2013). Since enrofloxacin is used in animal health, also ciprofloxacin will be found in waste water streams of animal farms.

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year		
Uses	Human medicine	
Spatial usage (by MS)		
Banned uses		
ERC code		
PEC_{fw} (µg/L)	Evaluation of the potential concentrations of four antibiotics (ciprofloxacin, sulfamethoxazole, trimethoprim, and erythromycin) throughout the rivers of Europe. This involved reviewing national consumption rates together with assessing excretion and	Johnson et al. (2015)

	sewage treatment removal rates. The modelled antibiotic concentrations were within the range of measurements reported previously in European effluents and rivers. With the expected scenario, **the predicted annual-average antibiotic concentrations ranged between 0 and 10 ng/l for 90% by length of surface waters**. In the worst case scenario concentrations could reach between 0.1 and 1 µg/l at the most exposed locations. As both predicted and observed sewage effluent concentrations were below reported effect levels for the most sensitive aquatic wildlife, no direct toxicity in rivers is expected.	
PEC_{fw} (µg/L)	7.5	(EMEA; 2006).
PEC_{fw} (µg/L)	0.139	(Besse and Garric, 2008)
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring data	MEC values (µg/l)
In Sc2 (inland whole water) data from 3 MS (54 sites) with 842 samples are available. 9% are quantified. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.037 (Sc2)
France	Canche River (urban impact) (Tlili et al., 2016)	0.007
Spain	Ter River downstream WWTP in Girona (Rodriguez-Mozaz et al., 2015)	0.072 (max)
USA	River in Maryland (He et al., 2015)	0.010 (upstream WWTP) 0.031 (max; downstream WWTP)

Worldwide monitoring data collected from 47 articles; in total 501 samples.	Sum of fluoroquinolones in surface water (Van Doorslaer et al., 2014)	0.026 (median)
China	Wenyu River (Zhang et al., 2014)	0.066 (max)
Poland	Gościcina and Reda Rivers (Wagil et al., 2014)	2.7 (max)
90 samples from 18 European countries	Ciprofloxacin in EU WWTP effluents (EU-wide monitoring survey) (Loos et al., 2013)	0.096 (mean) 0.264 (max)
Spain	Urban WWTP effluents in Girona (Gros et al., 2013)	0.147 (max)
France	Seine River; Charmoise River, downstream WWTP (Dinh et al., 2011)	0.017; 0.135
Italy	Surface water, River Po (Zuccato et al., 2010)	0.0088 (mean)
Italy	Surface water, River Arno (Zuccato et al., 2010)	0.019 (mean)
China	Tonghui River (Xiao et al., 2008)	0.010 (median); 0.020 (max)
China	Pearl River (Peng et al., 2008)	0.459 (max)
USA	Upper Tennessee River (Conley et al., 2008)	0.007 (median); 0.054 (max)
Finland	Vantaa River (Vieno et al., 2007)	0.025 (max)
USA	Streams downstream WWTPs (Batt et al., 2006)	0.170 (median); 0.360 (max)
France, Greece, Italy and Sweden	WWTP effluents (Andreozzi et al., 2003)	0.060 (median)

Italy	Po and Lambro River (Calamari et al., 2003)	0.020 (median); 0.026 (max)
Switzerland	WWTP effluent in Zuerich (Golet et al. 2002)	0.071 (mean)
USA	Surface water (Kolpin et al., 2002)	0.030 (max)

Analytical Methods

Ciprofloxacin

Method	**LOQ (µg/l)**	**Description / Reference**
SPE-LC-MS-MS	0.005	Filtration of water in case of visible particles; the pH is adjusted to 2.0; addition of tetrasodium ethylenediamine-tetraacetate dehydrate (NA_4EDTA 2 H_2O x 2 H_2O). Internal standard: $^{13}C_3$ ^{15}N-Ciprofloxacin. Extraction of 1 L water with Oasis HLB (60 mg). Positive ionisation; mass transitions: 332.2 - 314.2 (EPA, 2007)
SPE-LC-MS-MS	0.002	Extraction of 500 ml water; positive ionisation; mass transitions 332 > 288, 231 (Gros et al. (2009).
SPE-LC-MS-MS	0.018	Extraction of 100 ml water (Gros et al. (2012).
SPE-LC-MS-MS	0.006	Extraction of 100 ml water; positive ionisation; mass transitions 332 > 288, 245 (Gros et al. (2013).
SPE-LC-MS-MS	0.018	Extraction of 500 ml water; positive ionisation; mass transitions 332 > 288, 245 (Petrović et al. (2013).
SPE-LC-MS-MS	0.001	After filtration, to 800 mL of river water Na2EDTA (0.5% w/v) was added, acidified to pH 3.0 with hydrochloric acid (HCl), and then spiked with the surrogate standards before being passed through the Oasis HLB cartridges (500 mg) at a flow rate of approximately 5–10 mL/min. Elution with 1 mL methanol, and this eluate was cleaned-up with Oasis MAX cartridges; Ciprofloxacin recovery: 63 %; MRM transitions 332 > 288, 231 (Zhang et al., 2014).

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Ciprofloxacin	T		Not investigated	

The half-life time of fluoroquinolone antibiotics in surface water is approximately 10.6 days (Andreozzi et al., 2003; Van Doorslaer et al., 2014).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae			
Chlorella vulgaris	96 h, growth rate	EC10	1800
Cyanobacteria			
Anabaena flos-aquae	72 h, growth rate	EC10	4.47
Plants			
Lemna gibba	7 d, biomass	EC10	149
Myriophyllum spicatum	14 d	NOEC	980
Crustaceans			
Daphnia magna	21 d, reproduction	NOEC	4670

Source: ECOTOX 2013 (CH)

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value	AF	PNEC

		(µg/l)		value (µg/l)
$PNEC_{fw}$	72 h, EC10 (Growth rate, *Anabaena flos-aquae*)	4.47	50	0.089[a]
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				
$PNEC_{biota, hh}$				
$PNEC_{dw, hh}$				

[a] Source: Ecotox 2013 (CH)

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw}(MEC(P(95))/PNEC)	0.4[b]
RQ_{fw}(PEC/PNEC)c	84.2 [c]

[b] RQ is not reliable due to the low quality of MEC value

c PEC source from Initial assessment of eleven pharmaceuticals using the EMEA guideline in Norway (TA-2216/2006; ISBN 82-7655-295-1)

STE score

0.44 (Sc2; PNEC=0.089 µg/l)

Not reliable value

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Cyanide-Free (CAS N. 57-12-5)

Substance identity

EC name	
EC number	
CAS number	57-12-5
Molecular formula	HCN, CN^-
Molecular weight	27.03
Structure	
SMILES	C#N

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure	620 mmHg at 20°C (as HCN)	WFD – UK TAG Report, 2012[1]
Water solubility (mg/L)	1,000,000 at 25°C (as HCN) 10.9 mol/L (predicted)	WFD – UK TAG Report, 2012[1] https://comptox.epa.gov/dashboard/dsstoxdb/results?utf8=%E2%9C%93&search=Cyanide%2C+free
logK_{ow}	0.35–1.07 (as HCN)	WFD – UK TAG Report, 2012[1]

Environmental fate

Endpoint	Value	Source
Biodegradability	Biodegradation is an important transformation process for cyanide in natural surface waters and is dependent on such factors as cyanide concentrations, pH, temperature, availability of nutrients and acclimation of microbes.	WFD – UK TAG Report, 2012[1]
Bioaccumulation (BCF)	Experimental BCF values for rainbow trout range from 1.69–4.12.	WFD – UK TAG Report, 2012[1]

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year	11894 (2010) in CZ	CZ
Uses	Cyanides are used extensively in industry and are also emitted from car exhaust fumes. They also occur ubiquitously in the environment and are found in a range of aquatic organisms such as arthropods, macrophytes, fungi and bacteria. Cyanide is used in the following MS: CZ, IRL	WFD – UK TAG Report, 2012[1]
	Electroplating	CZ
Spatial usage (by MS)	Widespread use	
	In Northern Ireland used in very small number of industrial processes.	UK
Banned uses	-	
ERC code	-	
Fraction of tonnage to region	-	
PEC_{fw} (mg/L)	-	
PEC_{sed} (mg/kg dw)	-	
PEC_{biota} (mg/kg)	-	

Measured Environmental Concentrations

MS	**Source of monitoring data**	**MEC values**	**RBSP**
CZ	Waste water	2.5-11 μg/l (2015)	
UK	Monitored at 35 sites quarterly in water body's deemed at risk from Cyanide via permitted discharges.	Results show concentrations above the EQS at 3 sites. Results are limited by the LOD	

		limitations.	
14 (CZ, SI, EL, FR, DE, AT, ES, UK, IE, NL, PL, RO, SK, IT) Reported as cyanide in the databases	NORMAN DB, 2014[2]	$MEC_{95, whole}$: 1.07 µg/L $MEC_{95. dissolved}$: 5 µg/L	10 MS (RBSP EQS ECOSTAT – UBA report)[5] EQS set for cyanide ion and total (WRc, 2012)[6]
	WATERBASE, 2014[3]	$MEC_{95, whole}$: 20 µg/L $MEC_{95, dissolved}$: 20 µg/L	
	IPCheM[4]	MEC_{95}: 14 µg/L	

No data found in the dataset of the monitoring prioritisation 2014

Analytical Methods

Method	**LOQ (µg/l)**	**Description / Reference**
Free cyanide: CSN ISO 6703 Total cyanides: CSN 757415, CSN EN ISO 14403-2	Free cyanide: 5 µg/l Total cyanides: 1 – 5 µg/l	CZ
Spectrophotometric measure of total and free cyanide by molecular absorption	LOD: 0.1 µg/l LOQ: 0.5 µg/l	BE-Wallonia
SPEK (CFA), SIST EN ISO 14403-2:2013	LOD: 0.1 µg/L LOQ: 0.5 µg/L	Slovenia
Continuous flow analysis (CFA) with photometric detection	LOQ: 0.14 - 0.30 µg/l	Fraunhofer Institute (2017)
n.a.	LOD: 5 µg/l; Improved analytical capability would require significant investment and low prospect of	UK

	success.	

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Cyanide-free	T	-	-	-

Volatilisation and biodegradation are important transformation processes for cyanide in ambient waters. Hydrogen cyanide can be biodegraded by acclimated microbial cultures, but is usually toxic to unacclimated microbial systems at high concentrations (WFD- UK TAG Report, 2012[1]).

Hazard assessment

Ecotoxicology data

Trophic level	Endpoint	Value	Reference
Fish	Rainbow trout, 20 d, LOEC	5 µg/L	WFD- UK TAG Report (2012)[1]
Fish	***Lepomis macrochirus*, 289 d, total inhibiotin of spawning, LOEC**	**5.2 µg/L**	WFD- UK TAG Report (2012)[1]
Fish	*Salvelinus fontinalis*, egg production, NOEC	5.7 µg/L	WFD- UK TAG Report (2012)[1]
Aquatic Invertebrates	*Moinodaphnia macleayi*, 5 d, reproduction, NOEC	9.6 µg/L	WFD- UK TAG Report (2012)[1]
Aquatic Invertebrates	*Gammarus pseudolimnaeus,* 98 d, growth, NOEC	4 µg/L	WFD- UK TAG Report (2012)[1]
Aquatic Invertebrates	*Hydra viridissima*, 6 d, population growth,	110 µg/L	WFD- UK TAG Report (2012)[1]

	NOEC		
Algae	*Pseudokirchneriella subcapitata*, 72 h,growth rate and biomass, NOEC	10 µg/L	WFD- UK TAG Report (2012)[1]

Mammalian toxicology data

No information retrieved

PNEC derivation

PNEC	Endpoint	Endpoint value	AF	PNEC value
$PNEC_{fw}$	*Lepomis macrochirus*, 289 d, LOEC	5.2 µg/L	20	0.26 (µg/L)[a]
$PNEC_{sed}$	-	-	-	-
$PNEC_{biota,sec\ pois}$	-	-	-	-
$PNEC_{biota,\ hh}$	-	-	-	-
$PNEC_{dw,\ hh}$	-	-	-	50 (µg /L)[b]

N.R. Not required based on Koc and BCF values not reaching the trigger values required for sediment and biota assessment

[a] Value retrieved from WFD- UK TAG Report (2012)[1] . A more recent freshwater AA-EQS derivation of 5E-04 mg/l needs also to be considered.

[b] EU Drinking Water QS[7], refered to cyanide.

Risk Quotient (PEC/PNEC)

RQ	Value
RQ_{fw} (MEC 5-20)[c] and PNEC 0.5	10-40
RQ_{fw} (MEC 5-20)[c] and PNEC 0.26	19.2-76.8
RQ_{sed}	-
$RQ_{biota,sec\ pois}$	-
$RQ_{biota,\ hh}$	-

$RQ_{dw, hh}$	-

[c] **Dissolved fraction**

References

[1] Proposed EQS for Water Framework Directive Annex VIII substances: cyanide (free) (For consultation), Water Framework Directive - United Kingdom Technical Advisory Group (WFD-UKTAG), 2012. Available at http://www.wfduk.org/sites/default/files/Media/Cyanide_Final_.pdf

[2] NORMAN Database http://www.norman-network.net/?q=node/24

[3] WATERBASE Database http://www.eea.europa.eu/data-and-maps/data/waterbase-rivers-6

[4] IPCheM database at http://ipchem.jrc.ec.europa.eu/

[5] Ecological Environmental Quality Standards of "River Basin Specific Pollutants" in Surface Waters - Update and Development analysis of a European Comparison between Member States, by U. Irmer, F. Rau, J. Arle, U. Claussen, V. Mohaupt - Annex

[6] Contract No. 070311/2011/603663/ETU/D1 "Comparative Study of Pressures and Measures in the Major River Basin Management Plans' - Task 2c (Comparison of Specific Pollutants and EQS): Final Report". WRc Ref: UC8981/1 October 2012. Available at http://ec.europa.eu/environment/archives/water/implrep2007/pdf/P_M%20Task%202c.pdf

[7] COUNCIL DIRECTIVE 98/83/EC of 3 November 1998 on the quality of water intended for human consumption, Official Journal of the European Communities. Available at http://europa.eu/legislation_summaries/environment/water_protection_management/l28079_en.htm

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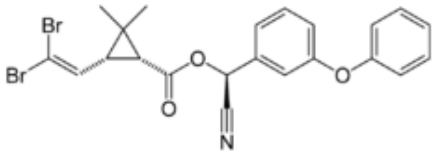
Deltamethrin (CAS N. 52918-63-5)

Substance identity

EC name	
EC number	
CAS number	52918-63-5
Molecular formula	$C_{22}H_{19}Br_2NO_3$
Molecular weight	505.21 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.0002	http://npic.orst.edu/factsheets/archive/Deltatech.html
Log K_{ow}	4.6 6.1	http://cegg-rcge.ccme.ca/download/en/170 http://npic.orst.edu/factsheets/archive/Deltatech.html

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	10240000	http://sitem.herts.ac.uk/aeru/ppdb/en/Reports/205.htm
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability		
Bioaccumulation (BCF)	1400	http://sitem.herts.ac.uk/aeru/ppdb/en/Reports/205.htm

See under bifenthrin.

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	PUSG usage data for 2015 noted 89097 hectares treated with 563 kg.	UK
Uses	Deltamethrin is approved as PPP in the EU (in agriculture to protect crops or kill livestock parasites). Deltamethrin is authorised in 28 MS's (AT, BE, BG, CY, CZ, DE, DK, EE, EL, ES, FI, FR, HR, HU, IE, IT, LT, LU, LV, MT, NL, PL, PT, RO, SE, SI, SK, UK).	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1197
Spatial usage (by MS)		
	Many products approved in UK re: PPP. Approved on a range of crops eg grain, pulses, storage structures, fruit, vegetables, ornamental garden plants, herbs and amenity vegetation. Also approved in relation to BPD in UK for use as an insecticide. Approved products primarily for ants and mosquito nets. Also some products approved under COPR for insecticide use. VMD use as a pour-on and spot on for cattle & sheep and also spot on for dogs. Scotland: deltamethrin used in fish farming for sea lice. Northern Ireland: used in agriculture.	UK
Banned uses		

ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 7 MS (2766 sites) with 28842 samples are available. Only 0.7% quantified samples. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.05 µg/l (Sc2)
UK	Monitored at approx. 500 sites as part of national catchment sensitive farming (CSF) & watch list programmes and WFD national surveillance programme.	Not detected in any samples.

See under bifenthrin.

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
GC-NCI-MS	0.00038	Extraction by ultrasound-assisted emulsification-extraction of a water-immiscible solvent (chloroform) in 20 mL water (Feo et al., 2010).

GC-NCI-MS	0.001	SPE of 1 L water (Elfman et al., 2011).
GC-ECD/MS	0.00006–0.00098 (LOD)	SPE (Zheng et al., 2016).
n.a.	0.005	Finland
n.a.	0.001 – 0.02	CZ

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Deltamethrin	B		ED	

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae			
Chlorella vulgaris	96 h	NOEC	470
Invertebrates			
Daphnia magna	21 d	NOEC	0.0041
Chironomus riparius	28 d	NOEC	0.010
Chironomus riparius	28 d	NOEC	0.0035
Gammarus pulex	21 d	NOEC	0.009
Tisbe battagliai	6 d	EC10	0.0161
Tisbe battagliai	6 d	EC10	0.0087
Tisbe battagliai	6 d	EC10	0.0281
Tisbe battagliai	6 d	LC10	0.0641
Fish			

Pimephales promelas	260 d	NOEC	0.017

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/l)	AF	PNEC value (µg/l)
$PNEC_{fw}$	28 d, NOEC *(Chironomus riparius)*	0.0035	50	0.00007
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				
$PNEC_{biota, hh}$				
$PNEC_{dw, hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	714 (Sc2)
RQ_{fw} (PEC/PNEC; PEC= 0.03 µg/l)	429
RQ_{fw} PEC/PNEC; PEC= 0.36 µg/l)	5143

Note: PEC values are taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based strategy for the prioritisation exercise under the Water Framework Directive,* https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

2.69 (Sc2; PNEC= 0.00007 µg/l)

References

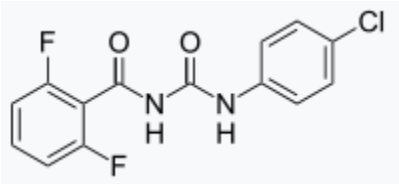
Elfman, L., Tooke, N.E., Patring, J.D.M.; Detection of pesticides used in rice cultivation in streams on the island of Leyte in the Philippines. Agricultural Water Management 101 (2011) 81– 87.

Feo, M.L., Eljarrat, E., Barceló, D.; A rapid and sensitive analytical method for the determination of 14 pyrethroids in water samples. Journal of Chromatography A, 1217 (2010) 2248–2253.

Zheng, S., Chen, B., Qiu, Q., Chen, M., Ma, Z., Yu, X. Distribution and risk assessment of 82 pesticides in Jiulong River and estuary in South China. Chemosphere 144 (2016) 1177–1192.

Diflubenzuron (CAS N. 35367-38-5)

Substance identity

EC name	
EC number	
CAS number	35367-38-5
Molecular formula	$C_{14}H_9ClF_2N_2O_2$
Molecular weight	310.68 $g \cdot mol^{-1}$
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.08	http://pmep.cce.cornell.edu/profiles/extoxnet/dienochlor-glyphosate/diflubenzuron-ext.html
Log K_{ow}	3.89	http://www.fao.org/fileadmin/templates/agphome/documents/Pests_Pesticides/JMPR/Evaluation02/Diflubenzuron_EvA2jj.pdf

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	4609 ml/g	Diflubenzuron assessment report, 2012
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)	65.2	Diflubenzuron assessment report, 2012
Biodegradability	Not readily biodegradable	Diflubenzuron assessment report, 2012
Bioaccumulation (BCF)	320	Diflubenzuron assessment report, 2012

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	5715 kg a.i. in 2015.	Romania
	2265 kg a.s. sold in DK in 2015 (increasing).	Denmark
	100.8 kg sold in 2015.	BE-Fl
	Pesticide usage data for 2015 for GB noted 970 hectares treated with 112 kg. There is one product approved under COPR which is an insecticide for professional use.	UK
Uses	Insecticide	
	Authorised in 20 MS; in 16 MS as a PPP (BE, BG, CY, CZ, EL, ES, HR, HU, IT, LT, NL, PL, PT, RO, SK, UK), in 3 MS as a biocide (DK, FI, SE), in 1 MS as a PPP and as a biocide (FR)	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1236 https://echa.europa.eu/it/information-on-chemicals/biocidal-products?p_p_id=echarevbiocidalproducts_WAR_echarevbiocidalproductsportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_echarevbiocidalproducts_WAR_echarevbiocidalproductsportlet_approval_id=0062-18 https://echa.europa.eu/it/information-on-chemicals/biocidal-active-substances?p_p_id=echarevbiocides_WAR_echarevbiocidesportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_echarevbiocides_WAR_echarevbiocidesportlet_rml_id=100.047.740
Spatial usage (by MS)	Removed from the PPP register in 2013; before that sold minor amounts. Still in use as biocide / veterinary use (against ectoparasite of minks).	Finland
	Larvae systemic insecticide	Romania
	Only approved for use against lice in mink farms in SE	Sweden
	Only approved for indoor use as biocide on lice in mink.	Denmark
	Uses registered for apples, horse-chestnuts,	Slovakia

	oak tree, and forest trees. Quantity unknown.	
	Admission for ornamental plants.	BE-Fl
	Currently 3 products approved for use in UK as plant protection products. Approved for use on a range of crops included amenity vegetation, fruit, vegetables, forestry, hedgerows, livestock housing, manure heap and refuse tips. In Scotland used as fish farm lice medicine.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 4 MS (415 sites) with 4725 samples are available. Only 2 samples are quantified. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.025 µg/l (Sc2)
England	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LCMS samples at approx. 80 sites.	0.0106 µg/l (mean based on 27 detect samples from 130 samples)

Analytical Methods

Method	LOD/LOQ (µg/l)	Description / Reference

LC-MS/ MS	0.1	Determination of diflubenzuron and the relevant metabolites CPU and DFBA in surface water based on LC-MS/MS (one ion transition) (Diflubenzuron assessment report; 2012).
n.a.	0.01	Finland
LC-MS/MS	0.04	Arysta Life Science
LC-MS/MS	0.005	UK

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Diflubenzuron	T			

No degradation at pH 5 or 7. Degradation to CPU and DFBA at pH 9 with DT_{50} =32.5 d (25°C). DT_{50} = 80 days of sunlight (at 40 °N) (Diflubenzuron assessment report, 2012).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Fish			
Oncorhynchus mykiss	21 d	NOEC	200
Invertebrates			
Mercenaria mercenaria	48 h, static	NOEC	320
Daphnia magna	21 d	NOEC	0.04
Mysidopsis bahia	28 d	NOEC	0.045
Algae			
Selenastrum capricornutum	72 h	EC50	>200

Data used for PNEC derivation

Source: EFSA 2012 and EU Report 2012

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	21-d NOEC (Reproduction, *Daphnia magna*)	0.04	50	0.0008
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				
$PNEC_{biota, hh}$				
$PNEC_{dw, hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	31.3 (Sc2)
RQ_{fw} (PEC/PNEC; PEC=13.62µg/l)	17025

STE score

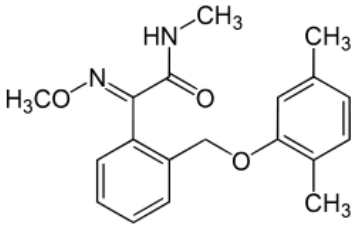
2.3 (Sc2; PNEC=0.0008µg/l)

References

Diflubenzuron assessment report under Directive 98/8/EC concerning the placing of biocidal products on the market; Product-type 18 (insecticides, acaricides and products to control other arthropods); 21 September 2012; Sweden.

Dimoxystrobin (CAS N. 149961-52-4)

Substance identity

EC name	
EC number	
CAS number	149961-52-4
Molecular formula	$C_{19}H_{22}N_2O_3$
Molecular weight	326.39 $g \cdot mol^{-1}$
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	4.3	http://sitem.herts.ac.uk/aeru/iupac/Reports/246.htm
Log K_{ow}	3.6	http://sitem.herts.ac.uk/aeru/iupac/Reports/246.htm

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	486.2 ml/g	EFSA, 2005
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)	Photolysis and partition to sediment was considered the main routes of dissipation of dimoxystrobin from the water phase in the outdoor water sediment study. A first order water phase $DT_{50water}$ = 15.3 d was calculated using only 0-58 d data.	EFSA, 2005
Biodegradability	Not readily biodegradable	EFSA, 2005
Bioaccumulation (BCF)	48	EFSA, 2005

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	Use: 8.485 in 2016.	CZ
	18.572 in 2015.	RO
	The PUSG data indicates 17717 hectares treated with 1797 kg for 2015.	GB
Uses	Dimoxistrobin is approved as PPP in EU (16 MS: AT, BE, BG, CZ, DE, EE, FR, HR, HU, LT, LU, LV, PL, RO, SK, UK)	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1251
	Strobilurin funcicide with the main uses in oilseed rape.	BASF, 2013
	Approval expiration date: 31/01/2019.	DG Sante
Spatial usage (by MS)	Not in PPP register, not sold as PPP in the 2000's. In Finland the compound is not use.	FI
	Uses registered for oil-seed rape, sunflower.	SK
	Admission for rapeseed.	BE-Fl
	Not approved in DK and SE.	SE; DK
	Two PPP products approved in UK currently. Approved for use on oilseed rape, durum wheat and wheat.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from only 1 MS (720 sites) with 6078 samples are available. 2.8% quantified samples. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.025 µg/l (Sc2) The MEC is unreliable due to the low quantity and quality of the monitoring data (see column on the left)
UK	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LC-MS samples at approx. 80 sites. In addition monitored at an additional approx. 500 sites.	Detects noted at 9 of these sites but infrequently. Lowest minimum concentration 0.0011 and highest max concentration 1.5 µg/l.

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
SPE-LC-MS-MS	0.025	Extraction of 10 ml water; elution with methanol (BASF, 2013)
LC-MS-MS	0.01	CZ
SPE-LC-MS-MS	0.01	BE-Wallonia
LC-MS-MS	0.001	England

Dimoxystrobin has mainly been analysed in food products (Lozowicka et al., 2014; Schurek et al., 2008; Wang et al., 2012; 2017).

Lozowicka et al. (2014) analysed pesticide residues (including dimoxystrobin) in grain (barley, oat, rye, and wheat) from Kazakhstan.

P, B, T, C, M, R, ED properties

Substance	Persistent (P)Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Dimoxystrobin	P and T			

Dimoxystrobin is stable to hydrolysis at all environmental relevant pHs. Photolysis may moderately contribute to the degradation of dimoxystrobin in water. Degradation of dimoxystrobin in water/sediment systems was very limited. Only 10-15 % of the applied dimoxystrobin degrades after 100 d. Disappearance from the water phase is mainly attributed to partition with sediment. Additionally an outdoor water sediment study and an outdoor mesocosm study in Germany were used to investigate the aquatic dissipation of dimoxystrobin. Photolysis and partition to sediment were considered the main routes of dissipation of dimoxystrobin from the water phase in the outdoor water sediment study. In the mesocosm study dimoxystrobin was applied in early May and a dissipation DT_{50} = 60 – 69 d was calculated for the water phase (EFSA, 2005).

The hydrolytic stability of dimoxystrobin was studied in sterile aqueous buffer solutions (pH 4, 5, 7, and 9) at 25 ºC and 50 ºC. Dimoxystrobin is stable at all environmental relevant pHs. Photolysis in water was investigated in two different studies. Photolysis may moderately contribute to the degradation of dimoxystrobin in water. Measured half life under continuous irradiation under laboratory conditions was 14.1 d (pond water) and 64.8 d (sterile buffer pH 7, extrapolated) (EFSA, 2005).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae & aquatic plants			
Pseudokirchneriella subcapitata	96 h	EC10	13.3
Invertebrates			
Daphnia magna	21 d, reproduction	NOEC	12.5
Daphnia magna	10 d, growth	NOEC	0.5
Chironomus riparius	28 d, emergence rate	NOEC	10
Fish			
Oncorhynchus mykiss	97 d, growth	NOEC	0.316

Oncorhynchus mykiss	97 d	NOEC	1
Acipenser ruthenus L.	7 d	NOEC (weight) NOEC (growth)	0.1 1
Oncorhynchus mykiss	28 d	NOEC	10
Pimephales promelas	36 d	NOEC	16

Data used for PNEC derivation

Source: UBA 2014 and EFSA 2005

Mammalian toxicology data

PNEC derivation

PNEC	**Endpoint**	**Endpoint value (µg/L)**	**AF**	**PNEC value (µg/L)**
$PNEC_{fw}$	97-d NOEC (body length, ELS*, *Oncorhynchus mykiss*)	0.316	10	0.0316
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	**Value**
RQ_{fw} (MEC(P(95))/PNEC)	0.79 (Sc2)
RQ_{fw} (PEC/PNEC; PEC=16.42 µg/l)	519.6

Note: PEC value is taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based*

strategy for the prioritisation exercise under the Water Framework Directive, https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

0 (Sc2; PNEC=0.0316 µg/l)

References

BASF, 2013. Method for the determination of BAS 505 F, 505M98 (Reg.No. 360056), 505M01 (Reg.No. 358104), 505M08 (Reg.No. 354562) and 505M09 (Reg.No. 354563) in surface water and groundwater by LC-MS/MS; BASF Method Number L0191/01

EFSA, 2005. Conclusion regarding the peer review of the pesticide risk assessment of the active substance dimoxystrobin; EFSA Scientific Report (2005) 46, 1-82.

Lozowicka, B., Kaczynski, P., Paritova, A.E., Kuzembekova, G.B., Abzhalieva, A.B., Sarsembayeva, N.B., Alihan, K. 2014. Pesticide residues in grain from Kazakhstan and potential health risks associated with exposure to detected pesticides. Food and Chemical Toxicology 64 (2014) 238–248.

Schurek, J., Vaclavik, L., Hooijerink, H., Lacina, O., Poustka, J., Sharman, M., Caldow, M., Nielen, M.W.F., Hajslova, J. 2008. Control of Strobilurin Fungicides in Wheat Using Direct Analysis in Real Time Accurate Time-of-Flight and Desorption Electrospray Ionization Linear Ion Trap Mass Spectrometry. Anal. Chem. 2008, 80, 9567–9575.

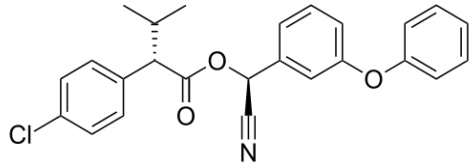
Szöcs, E., Brinke, M., Karaoglan, B., Schäfer, R.B. 2017. Large Scale Risks from Agricultural Pesticides in Small Streams. Environ. Sci. Technol. 2017, 51, 7378−7385.

Wang, J., Chow, W., Leung, D., Chang, J. 2012. Application of Ultrahigh-Performance Liquid Chromatography and Electrospray Ionization Quadrupole Orbitrap High-Resolution Mass Spectrometry for Determination of 166 Pesticides in Fruits and Vegetables. J. Agric. Food Chem. 2012, 60, 12088−12104.

Wang, J., Chow, W., Chang, J., Wong, J.W. 2017. Development and Validation of a Qualitative Method for Target Screening of 448 Pesticide Residues in Fruits and Vegetables Using UHPLC/ESI Q‐Orbitrap Based on Data-Independent Acquisition and Compound Database. J. Agric. Food Chem. 2017, 65, 473−493.

Esfenvalerate (CAS N. 66230-04-4)

Substance identity

EC name	
EC number	
CAS number	66230-04-4
Molecular formula	$C_{25}H_{22}ClNO_3$
Molecular weight	419.91 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	<0.001 at pH 5, 20 °C; nearly insoluble in water	EFSA, 2014
Log K_{ow}	6.24	EFSA, 2014

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	251700 ml/g	EFSA, 2014
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	
Bioaccumulation (BCF)	3369	http://www.rivm.nl/bibliotheek/rapporten/601716017.pdf EFSA, 2014

See under bifenthrin.

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	PUSG usage data for 2015 indicates 246807 hectares treated with 919 kg.	GB
Uses	Esfenvalerate is approved as PPP in the EU (in agriculture to protect crops or kill livestock parasites). Esfenvalerate is authorised in 25 MS (AT, BE, BG, CY, CZ, DE, DK, EL, ES, FI, FR, HR, HU, IE, IT, LT, LU, LV, NL, PL, PT, RO, SE, SK, UK).	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1286
	Only uses as insecticide may be authorised.	http://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:32011R0540&from=EN
Spatial usage (by MS)		
	10 products approved in the UK in relation to PPP. Approved for use on a wide range of crops including cereal, vegetables, turf, and grassland.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 4 MS (1152 sites) with 8661 samples are available. Only 0.5% quantified samples. In Sc3 (inland whole water; PNEC=0.0001 µg/l) data from only 2 MS (26 sites) with 87 samples are available. 52.9% quantified samples. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.05 µg/l (Sc2) MEC(P95)= 0.017 µg/l (Sc3)
UK	Monitored at approx. 600 sites as part of national catchment sensitive farming (CSF) & watch list programmes and WFD national surveillance programme.	Not detected in any samples.

See under bifenthrin.

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
GC-NCI-MS	0.0001	Extraction by ultrasound-assisted emulsification-extraction of a water-immiscible solvent (chloroform) in 20 mL water (Feo et al., 2010).
GC-MS	0.06	SPE of water (Bereswill et al., 2013).
GC-ECD	0.001	Surface water and drinking water analysis (EFSA, 2014).

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Esfenvalerate	B and T			

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae			
Pseudokirchneriella subcapitata	48 hr, growth rate	NOEC	1.0
Invertebrates			
Daphnia magna	21 d, reproduction	NOEC	0.052
Daphnia magna	21 d, reproduction	NOEC	0.056
Chironomus riparius	28 d	NOEC	0.16
Fish			
Lepomis macrochirus	30 d, mortality	NOEC	0.092
Lepomis macrochirus	60 d, mortality	NOEC	0.052
Lepomis macrochirus	90 d, mortality	NOEC	0.010
Oncorhynchus mykiss	21 d, mortality	NOEC	0.001
Pimephales promelas	260 d, survival	NOEC	0.090
Salmo gairdneri	21 d	NOEC	0.001
Mesocosm study			
Aquatic insects	-	NOEC	0.001

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	21-day, mortality (*Oncorhynchus mykiss*)	0.001	10	0.0001
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (for MEC(P(95)) and PNEC=0.0001 µg/l)	500 (Sc2) 170 (Sc3)
RQ_{fw} (for PEC= 0.0634µg/l and PNEC= 0.0001 µg/l)	634
RQ_{fw} (for PEC= 0.0054µg/l and PNEC= 0.0001 µg/l)	54

Note: PEC values are taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based strategy for the prioritisation exercise under the Water Framework Directive,* https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE scores

2.56 (Sc2)

1.94 (Sc3)

References

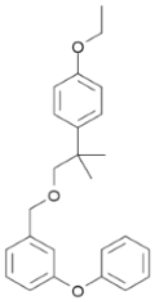
Bereswill, R., Streloke, M., Schulz, R.; Current-used pesticides in stream water and suspended particles following runoff: Exposure, effects, mitigation requirements. Environ. Toxicol. Chem. 32 (2013) 1254-1263.

EFSA, 2014. Conclusion on the peer review of the pesticide risk assessment of the active substance esfenvalerate. EFSA Journal 2014; 12(11): 3873.

Feo, M.L., Eljarrat, E., Barceló, D.; A rapid and sensitive analytical method for the determination of 14 pyrethroids in water samples. Journal of Chromatography A, 1217 (2010) 2248–2253.

Etofenprox (CAS N. 80844-07-1)

Substance identity

EC name	
EC number	407-980-2
CAS number	80844-07-1
Molecular formula	$C_{25}H_{28}O_3$
Molecular weight	376.49 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)	8.13×10^{-7}	Etofenprox assessment report, 2013
Water solubility (mg/L)	0.0225	Etofenprox assessment report, 2013
logK_{ow}	6.9	Etofenprox assessment report, 2013

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	28524 ml/g	Etofenprox assessment report, 2013
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	Etofenprox assessment report, 2013
Bioaccumulation (BCF)	3951 L/kg	Etofenprox assessment report, 2013

Hydrolysis of etofenprox was investigated in aqueous buffered solutions (pH: 4, 7 and 9) at 50 ° C. Etofenprox was stable (< 10 % degradation) in all three experimental

conditions. Therefore, chemical hydrolysis is not expected to contribute to the environmental degradation of etofenprox. Aqueous photolysis of etofenprox under artificially simulated sunlight (Suntest CPS, Herareus, Xe lamp) was investigated in buffered solutions (pH 7) and in natural pond water at 25 ° C. Photolysis of etofenprox is relatively rapid in both systems ($DT_{50\ buffered\ pH\ 7}$ = 4.7 days equivalent to $DT_{50\ 35^\circ N}$ = 10.4 days; $DT_{50\ pond}$ = 7.9 days equivalent to $DT_{50\ 35^\circ N}$ = 17.5 days). Major aqueous photolysis metabolites were α-CO (max 63.6 % at pH 7 and max. 37.8 % in pond water after 15 days, end of the study) and PENA (max. 12 % at pH 7 and max. 14.4 % in pond water after 15 days, end of study) (EFSA, 2008).

Dissipation/ degradation of etofenprox in water/sediment systems was investigated in two systems (pH_{water} = 6.1 – 7.8[27]; OC 5.1 – 7.3 %, clay 18.1 – 19.4 %). Rapid partition of etofenprox to the sediment occurs during the first seven days. The meeting of experts agreed on the half-lives calculated for etofenprox in the whole system ($DT_{50\ whole\ system}$ = 6.5 days – 20.1 days). Metabolite 4'- OH was identified as a major metabolite (max. 12.2 – 21.4 %) in the sediment phase of both systems (EFSA, 2008).

This metabolite degraded in the whole water/sediment system with a half-life of 21.8 - 57 days (EFSA, 2008).

The meeting of experts discussed the need to consider aqueous photolysis and photolysis metabolites for the EU risk assessment. From the results of the aqueous photolysis study and the mesocosm study the meeting concluded that photolysis could be a relevant process of etofenprox transformation in the environment. However, the results of the water/sediment study under light/dark cycles were considered inconclusive, possibly due to the strong sorption of the active substance to the sediment (EFSA, 2008).

Additional information on pyrethroids: see under bifenthrin.

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year	0.550 in 2015.	RO
Uses	Etofenprox is authorised in 18 MS; in 10 MS as a PPP (BG, CZ, EL, ES, HU, MT, PL, RO, SK, UK), in 4 MS as a PPP and as a biocide (AT, DE, FR, IT) and in 4 MS as a biocide (DK, LU, SE, SI)	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1307 https://echa.europa.eu/it/information-on-chemicals/biocidal-active-substances?p_p_id=echarevbiocides_WAR_echarevbiocidesportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_echarevbiocides_WAR_echarevbiocidesportlet_rml_id=100.100.942 https://echa.europa.eu/it/information-on-chemicals/biocidal-products?p_p_id=echarevbiocidalproducts_WAR_echarevbiocidalproductsportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_echarevbiocidalproducts_WAR_echarevbiocidalproductsportlet_approval_id=0030-18

	Insecticide.	
Spatial usage (by MS)	Not in PPP register, not sold as PPP in the 2000's. Still in use as biocide against ants (in outdoor close to buidings). In Finland the use is very limited and used amounts small => unlike to detect from water.	FI
	Pyrethroid insecticide –.; moderate use in Romania	RO
	Only approved against bed bugs in SE.	SE
	No registered sale from 2012 to 2015. It was approved as biocide for combatting ants outdoor in 2012. Expect use as biocide in the future.	DK
	Uses registered for forest trees, oak tree, pine, spruce, oil-seed rape.	SK
	No use in BE.	BE-Fl
	One product currently approved for use in UK as a PPP product. Approved for use on oilseed rape. No data available on extent of usage.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring	MEC values

	data	
In Sc2 (inland whole water) data from 3 MS (91 sites) with 1116 samples are available. Only 10 samples are quantified. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.01 µg/l (Sc2)

See under bifenthrin.

Analytical Methods

Albaseer et al. (2010) give an overview of sample preparation and extraction of synthetic pyrethroids from water, sediment and soil.

Method	**LOQ (µg/l)**	**Description / Reference**
SPE-GC-ECD/MS or GC-MS	0.00006–0.00098 (LOD)	Investigation of the distribution and risk assessment of 82 pesticides in Jiulong River and estuary (surface waters) in South China. SPE with ENVI-Carb column and LC-NH_2 column. (Zheng et al., 2016).
GC-MS	0.05 (drinking and ground water) 0.01 (surface water)	Monitoring of residues of etofenprox and α-CO in water (EFSA, 2008; Etofenprox assessment report, 2013).

P, B, T, C, M, R, ED properties

Substance	**Persistent (P) Bioaccumulative (B) Toxic (T)**	**Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)**	**Endocrine Disruptive (ED)**	**Comment**
Etofenprox	B and T	R		

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Fish			
Oncorhynchus mykiss	21d, semi-static	Mortality and growth, NOEC	2.1
Brachydanio rerio	40 d, flow-through	Mortality and development, NOEC	25
Invertebrates			
Daphnia magna	21 d, semi-static	Reproduction, NOEC	0.054
Algae			
Pseudokirchneriella subcapitata	72 h, static	Biomass, NOEC	56.25
Sediment dwelling organisms			
Chironomus riparius	25 d, static water-sediment system, spiked water	Emergence, Development, NOEC	3.8

Data used for PNEC derivation

Source: EU-RAR 2013 and EFSA 2008

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/l)	AF	PNEC value (µg/l)
$PNEC_{fw}$	21 d, semi-static, reproduction (*Daphnia magna*)	0.054	50	0.001
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				

$PNEC_{dw, hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	10 (Sc2)
RQ_{fw} (PEC/PNEC)	8300

Note: PEC value is taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based strategy for the prioritisation exercise under the Water Framework Directive,* https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

2.2 (Sc2; PNEC=0.001 µg/l)

References

Albaseer, S.S., Nageswara Rao, R., Swamy, Y.V., Mukkanti, K. 2010. An overview of sample preparation and extraction of synthetic pyrethroids from water, sediment and soil; Journal of Chromatography A, 1217 (2010) 5537–5554.

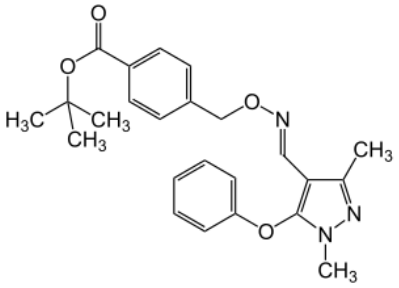
EFSA, 2008. Conclusion on pesticides peer review. Conclusion regarding the peer review of the pesticide risk assessment of the active substance etofenprox. 19 December 2008. http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2009.213r/epdf.

Etofenprox assessment report under Regulation 528/2012/EU concerning the making available on the market and use of biocidal products; Product-type 18 (Insecticide); September 2013, Austria.

Zheng, S., Chen, B., Qiu, Q., Chen, M., Ma, Z., Yu, X. 2016. Distribution and risk assessment of 82 pesticides in Jiulong River and estuary in South China. Chemosphere 144 (2016) 1177–1192.

Fenpyroximate (CAS N. 134098-61-6)

Substance identity

EC name	
EC number	
CAS number	134098-61-6
Molecular formula	$C_{24}H_{27}N_3O_4$
Molecular weight	421,49 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.023	EFSA, 2013
Log K_{ow}	5.0	EFSA, 2013

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	52067	EFSA, 2013
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	EFSA, 2013
Bioaccumulation (BCF)	1601	EFSA, 2013

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	0.235 in 2015.	RO
	0.006 in 2015.	DK
Uses	Fenpyroximate is authorised as PPP in 18 MS (AT, BE, BG, CY, CZ, DE, DK, EL, ES, FR, HU, IT, PL, PT, RO, SE, SI, SK)	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1352
Spatial usage (by MS)	Not in PPP register, not sold as PPP in the 2000's. In Finland the compound is not use.	FI
	Approved for use on apple, pear and in green houses.	SE
	Uses registered for strawberries, soya.	SK
	Admission for fruit trees.	BE-Fl
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from only 1 MS (35 sites) with 1506 samples are available. Only1 quantified sample. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.01 µg/l (Sc2)

	UK	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LC-MS samples at approx. 80 sites.	Not detected in any of the 1700 samples taken at these sites.

Analytical Methods

Fenpyroximate has mainly been analysed in food products (Banerjee et al., 2009; Herrera Lopez et al., 2016; Zhao et al., 2014).

Method	LOQ (µg/l)	Description / Reference
HPLC-MS SIM	0.1	(EFSA, 2013)
LC-MS-MS	0.005 (LOD)	England

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Fenpyroximate	P and B and T			

In laboratory incubations in dark aerobic natural sediment water systems (only pyrazole ring ^{14}C radiolabelled), fenpyroximate exhibited moderate persistence, forming the major metabolites M-3 (max. ca. 20.8 % AR in water), M-11 (max. 21 % AR in sediment), and M-8 (max. 28 % AR in water). In satisfactory field dissipation studies carried out at four sites in Germany (spray application to the soil surface on bare soil plots in early summer) fenpyroximate exhibited low to moderate persistence (EFSA, 2013).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)

Algae			
Scenedesmus subspicatus	72 h, static	NOEC	1
Fish			
Oncorhynchus mykiss	long-term, 21 d flow through	NOEC	0.19
Pimephales promelas	long-term, 34 d, flow through	NOEC	0.1
Invertebrates			
Daphnia magna	long-term, 21 d, semi-static	NOEC	0.68
Chironomus riparius	long-term, 28 d, static	NOEC	10
Microcosm study			
Zooplancton	28 d	NOEC	1

Data used for PNEC derivation

Source: EFSA 2008

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	34 d, NOEC (*Pimephales promelas*)	0.1	10	0.01
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	1 (Sc2) [a]
RQ_{fw} (PEC/PNEC; PEC=4.4 µg/l)	440

[a] RQ is not reliable due to the low quality of MEC value

Note: PEC value is taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based strategy for the prioritisation exercise under the Water Framework Directive,* https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

0 (Sc2; PNEC=0.01 µg/l)

Not reliable value

References

EFSA, 2013. Conclusion on pesticides peer review. Conclusion on the peer review of the pesticide risk assessment of the active substance fenpyroximate; EFSA Journal 2013;11(12):3493; http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2013.3493/epdf.

Herrera Lopez, S., Lozano, A., Sosa, A., Dolores Hernando, M., Fernandez-Alba, A.R. 2016. Screening of pesticide residues in honeybee wax comb by LC-ESI-MS/MS. A pilot study. Chemosphere 163 (2016) 44-53.

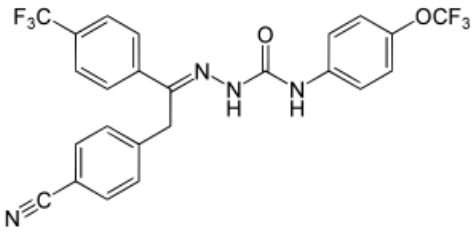
Zhang, X., Liu, X., Luo, Y., Zhang, M. 2008. Evaluation of water quality in an agricultural watershed as affected by almond pest management practices. Water Research 42 (2008) 3685 – 3696.

Banerjee, K., et al. 2009. Multiresidue Determination and Uncertainty Analysis of 87 Pesticides in Mango by Liquid Chromatography-Tandem Mass Spectrometry. J. Agric. Food Chem. 2009, 57, 4068–4078.

Zhao, M.-A., Feng, Y.-N., Zhu, Y.-Z., Kim, J.-H. 2014. Multi-residue Method for Determination of 238 Pesticides in Chinese Cabbage and Cucumber by Liquid Chromatography−Tandem Mass Spectrometry: Comparison of Different Purification Procedures. J. Agric. Food Chem. 2014, 62, 11449−11456.

Metaflumizone (CAS N. 139968-49-3)

Substance identity

EC name	
EC number	
CAS number	139968-49-3
Molecular formula	$C_{24}H_{16}F_6N_4O_2$
Molecular weight	506.40 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.00179	EFSA, 2013
Log K_{ow}	4.2-4.9	EFSA, 2013

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	30714 mL/g	EFSA, 2013
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	EFSA, 2013
Bioaccumulation (BCF)	7800 - 8100	EFSA, 2013

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source

Tonnes/year	0.054 in 2015.	RO
Uses	Metaflumizone is approved as PPP in the EU (13 MS: AT, BG, CY, EL, ES, HR, HU, IT, LT, PL, PT, RO, SI). The approval is in progress for NL.	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1553
Spatial usage (by MS)	Not in PPP register, not sold as PPP in the 2000's. In Finland the compound is not use.	FI
	Previously used against fleas, ticks and demodex in spot-on product for dogs. The vet prod was de-registred 2015. No use as PPP or biocidal products.	SE
	Not approved in DK.	DK
	Fleas and tick control in dogs.	SK
	No use in BE.	BE-Fl
	Used in livestock farming in Northern Ireland.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

No data found in the dataset of the monitoring prioritisation 2014.

MS	Source of monitoring data	MEC values
UK	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LC-MS samples at approx. 80 sites.	Only detected once out of the approx. 1700 samples taken at these sites (0.14 µg/l).

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
LC-MS/MS	0.025	Metaflumizone E-isomer and Z-isomer can be monitored in drinking water and surface water by LC-MS/MS. The validation was performed using the 2nd mass transition 507>178 m/z as well as primary mass transition 507>287 m/z for quantitation (EFSA, 2013).
LC-MS/MS	0.05	LLE from 50 ml water with dichloromethane; LC-MS/MS transitions: 507> 287, 178 m/z (BASF, 2003).
EN ISO 11369[25] modif.	0.01/0.02	Slovenia (SPE – solid-phase extraction)
LC-MS	0.005	Water sample preconcentration by SPE followed bu Ultra-High-Definition (UHD) Accurate-Mass Quadrupole Time-of-Flight (Q-TOF) MS. England

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Metaflumizone	vP, vB and T			

Metaflumizone was hydrolysed in water at pH < 7 with first order DT_{50} values ranging from 5.37 to 5.95 d (pH 4) and from 27.2 to 27.5 d (pH 5) at 25°C. Metaflumizone was stable to hydrolysis at pH 7 and 9 under the same conditions. Metaflumizone was photolysed in sterile water at pH 9 following 15 days of artificial irradiation, with single first order DT_{50} values ranging from 2.4 and 4.1 days (EFSA, 2013).

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity

[25] EN ISO method 11369 "Determination of selected plant treatment agents in water by high performance liquid chromatography with UV detection after solid-liquid extraction" from 1997 uses SPE with RP-C18 sorbent followed by HPLC-UV detection.

			(µg/L)
Fish			
Oncorhynchus mykiss	93 d (flow through)	NOEC	1.47
Danio rerio	148 d (static, with sediment)	NOEC	15
Invertebrates			
Daphnia magna	21 h (flowthrough)	NOEC	1.47
Americamysis bahia	28 d (flowthrough)	NOEC (survival/repro.)	0.654
Chironomus riparius	28 d (static water sediment study, with spiked water)	NOEC	2.56
Algae			
Pseudokirchneriella subcapitata	72 h	EC10	>313

Data used for PNEC derivation

Source: EFSA 2013 and CLH Report 2016

Mammalian toxicology data

PNEC derivation

PNEC	**Endpoint**	**Endpoint value (µg/L)**	**AF**	**PNEC value (µg/L)**
$PNEC_{fw}$	28-d NOEC (Reproduction/survival for *A. bahia*)	0.654	10	0.0654
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				

$PNEC_{biota, hh}$				
$PNEC_{dw, hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	**Value**
RQ_{fw}	n/a
RQ_{fw} (PEC/PNEC; PEC=0.3 µg/l)	4.6

STE scores

n/a (since missing data)

References

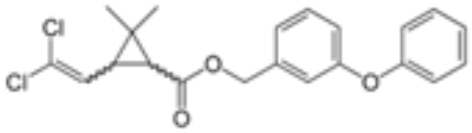
BASF, 2003. Method for the determination of BAS 320 I (E- and Z-isomer) and its metabolites in tap- and surface water. BASF method 534/0.

EFSA, 2013. Conclusion on pesticides peer review. Conclusion on the peer review of the pesticide risk assessment of the active substance metaflumizone. EFSA Journal 2013;11(10):3373; http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2013.3373/epdf.

EN ISO 11369, 1997. Determination of selected plant treatment agents in water by high performance liquid chromatography with UV detection after solid-liquid extraction (ISO 11369; 1997).

Permethrin (CAS N. 52645-53-1)

Substance identity

EC name	
EC number	
CAS number	52645-53-1
Molecular formula	$C_{21}H_{20}Cl_2O_3$
Molecular weight	391.28 g/mol
Structure	
SMILES	

Physico-chemical Properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.006 - 0.2; nearly insoluble in water	
Log K_{ow}	6.1	

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}		
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	
Bioaccumulation (BCF)	570	

See under bifenthrin.

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year		
Uses	Permethrin is not approved anymore as PPP in the EU (in agriculture to protect crops or kill livestock parasites).	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1687
	The authorisations for permethrin as a PPP were withdrawn by a Commission decision in 2000:	http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32000D0817
	Permethrin is approved in IE for use in biocidal products, wood preservatives (Product Typ 8), insecticides, acaricides and products to control other arthropods (Product Typ 18). Substance explicitly approved as biocide only.	http://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32014R1090&from=EN https://echa.europa.eu/it/information-on-chemicals/biocidal-active-substances?p_p_id=echarevbiocides_WAR_echarevbiocidesportlet&p_p_lifecycle=0&p_p_col_id=column-1&p_p_col_pos=1&p_p_col_count=2&_echarevbiocides_WAR_echarevbiocidesportlet_rml_id=100.052.771
Spatial usage (by MS)		
	No PPP products approved in the UK. Several products approved under COPR in relation to biocide use as used as an insecticide.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 7 MS (2431 sites) with 29730 samples are available. Only 0.4% quantified samples. In Sc3 (inland whole water; PNEC=0.00047µg/l) data from 4 MS (74 sites) included 117 samples. 98.3% quantified samples. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.025 µg/l (Sc2) MEC(P95)= 0.09 µg/l (Sc3)
UK	Monitored at 77 sites quarterly in water body's deemed at risk from permethrin via permitted discharges. At none of the sites assessed were the averages above the UK EQS.	A few detects noted with the maximum concentration detected 0.00756 µg/l

See under bifenthrin.

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
LLE followed by HRGC/HRMS	0.000044 (LOD)	US EPA method 1699 (2007)
LLE-GC-MS	0.0015	LLE of 1 L water; silica gel clean-up. (Kupper et al., 2006).
n.a.	0.005	Finland
n.a.	0.0001	England

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Permethrin	PT	-	-	-

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Algae			
Pseudokirchneriella subcapitata	72 h, cell density	NOEC	< 3.1
Invertebrates			
Daphnia magna	21 d, reproduction	NOEC	0.0047
Fish			
Zebrafish	35 d, survival	NOEC	0.41
Pimephales promelas	32 d, survival	NOEC	0.66
Cyprinodon variegatus	28 d, survival	NOEC	10

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$	21 d, reproduction (*Daphnia magna*)	0.0047	10	0.00047
$PNEC_{sed}$				

$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	**Value**
RQ_{fw} (for MEC(P(95)) and PNEC= 0.00047µg/l)	53.2 (Sc2) 191 (Sc3)
RQ_{fw} (PEC/PNEC)	n/a

STE scores

2.41 (Sc2)

2.29 (Sc3)

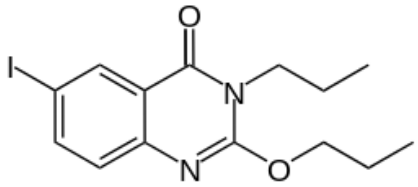
References

EPA method 1699, 2007. Pesticides in Water, Soil, Sediment, Biosolids, and Tissue by HRGC/HRMS. U.S. Environmental Protection Agency; EPA-821-R-08-001. December 2007.

Kupper, T.; Plagellat, C., Braendli, R.C., de Alencastro, L.F., Grandjean, D., Tarradellas, J.; Fate and removal of polycyclic musks, UV filters and biocides during wastewater treatment; Water Research 40 (2006) 2603-2612.

Proquinazid (CAS N. 189278-12-4)

Substance identity

EC name	
EC number	
CAS number	189278-12-4
Molecular formula	$C_{14}H_{17}IN_2O_2$
Molecular weight	372,2 g/mol
Structure	
SMILES	

Physico-chemical properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.97	EFSA, 2009
Log K_{ow}	5.5	EFSA, 2009

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	12870 mL/g	EFSA, 2013
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)	In water / sediment systems, proquinazid partitioned rapidly into the sediment (DissT50 < 1 d). However, it is moderately to highly persistent in the total system (DT50 = 36.5 – 136 d).	EFSA, 2013
Biodegradability	Not readily biodegradable	EFSA, 2013
Bioaccumulation (BCF)	821	EFSA, 2013

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source

Tonnes/year	5 in 2015.	RO
	PUSG data for 2015 indicates 285376 hectares treated in 2015 with 6405 kg.	GB
Uses	Proquinazide is a local systemic fungicide that inhibits the pathway for appressinogenesis in fungi. The active substance is used to combat powdery mildew in agriculture, fruit growing and viticulture. Proquinazid is approved as PPP in the EU (24 MS: AT, BG, CY, CZ, DE, EE, EL, ES, FI, FR, HR, HU, IE, IT, LT, LU, LV, MT, PL, PT, RO, SI, SK, UK). The approval is in progress for SE	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1779
	Fungicide.	
Spatial usage (by MS)	Use as plant protection chemical in Finland (one of the most used fungicides for cereals).	FI
	Approved as PPP against mildew on cereal since 2017-03-30.	SE
	Not approved in DK.	DK
	Uses registered on wheat, barley.	SK
	No use in BE.	BE-Fl
	Seven products approved in UK as PPP product. Approved for use on barley, wheat, oats, rye and triticale.	UK
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from only 1 MS (31 sites) with 1285 samples are available. No quantified	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.01 µg/l (Sc2)

samples. Sc3 was not developed since data scarcity. Data quality is not good.		
UK	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LC-MS samples at approx. 80 sites.	Only detected once out of the approx. 1700 samples taken at these sites (0.002 µg/l).

Analytical Methods

Method	LOQ (µg/l)	Description / Reference
GC-MS	0.1	Proquinazid and also the metabolites IN-MM986, IN-MM671 and IN-MM991 can be determined in surface, ground and drinking water by GC-MS. Quantification was on the m/z 288 ion for proquinazid and IN-MM986, and m/z 162 for INMM671 and IN-MM991 (EFSA, 2009).
LC-MS-MS	0.001	England

P, B, T, C, M, R, ED properties

Substance	Persistent (P)Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Proquinazid	vP, B and T			

Proquinazid and all the metabolites investigated were stable to hydrolysis (pH 4, 7 and 9). In the aqueous photolysis study proquinazid is rapidly photolysed (DT50 < 1 h) (EFSA, 2013).

Hazard assessment

Ecotoxicology data

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value	AF	PNEC value
$PNEC_{fw}$				0.18 µg/l
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	0.05 (Sc2) [a]
RQ_{fw} (PEC/PNEC)	7.28

[a] RQ is not reliable due to the low quality of MEC value

STE scores

0 (Sc2; PNEC=0.18 µg/l)

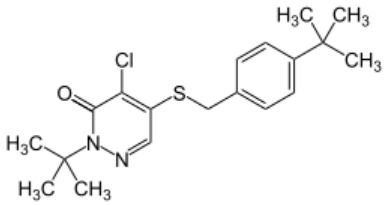
Not reliable value

References

EFSA, 2013. Conclusion on pesticides peer review. Conclusion on the peer review of the pesticide risk assessment of the active substance proquinazid; EFSA Journal 2009; 7(10):1350; http://onlinelibrary.wiley.com/doi/10.2903/j.efsa.2009.1350/epdf.

Pyridaben (CAS N. 96489-71-3)

Substance identity

EC name	
EC number	
CAS number	96489-71-3
Molecular formula	$C_{19}H_{25}ClN_2OS$
Molecular weight	364,93 g/mol
Structure	
SMILES	

Physico-chemical properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	0.022	EFSA, 2010
Log K_{ow}	6.37	EFSA, 2010

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}	66503 mL/g	EFSA, 2010
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability	Not readily biodegradable	EFSA, 2010
Bioaccumulation (BCF)	< 48	EFSA, 2010

In soil laboratory incubations under aerobic conditions in the dark, pyridaben exhibits moderate to high persistence forming the minor (<10 % applied radioactivity (AR)) metabolites PB-4 (max. 7.6 % AR, persistence endpoints not available) and PB-7 (max. 8.5 % AR, exhibiting low to moderate persistence). Under the conditions of a laboratory soil photolysis study, degradation of pyridaben was enhanced compared to that which occurred in the dark…Pyridaben is considered immobile in soil. (EFSA, 2010).

Field dissipation studies were available from two sites in Denmark and two sites in Spain (spray application to the soil surface on bare soil plots in April, except one of the Spanish trials where an October application was made). At the site with the October application date, pyridaben exhibited high persistence (single first order pattern of decline), i.e. a comparable pattern of persistence to that exhibited in the laboratory incubations. In the trials with the April applications, photolysis appears to be playing its part in the measured decline as a biphasic pattern of decline was observed. In these spring application trials pyridaben exhibited moderate persistence. (EFSA, 2010).

In laboratory incubations in dark aerobic natural sediment water systems, pyridaben exhibited moderate persistence. Under the conditions of a laboratory aqueous photolysis study pyridaben was rapidly degraded (within hours) to form the major metabolites W-1 and B-3 which were also rapidly degraded under the conditions of the test (EFSA, 2010).

The potential for groundwater contamination consequent to these uses from pyridaben or its metabolites PB-22, PB-4 and PB-7 above the parametric drinking water limit of 0.1µg/L was assessed as low (EFSA, 2010).

Environmental exposure assessment

Predicted Environmental Concentration

	Description	**Source**
Tonnes/year	0.023 in 2015	RO
Uses	Pyridaben is authorised as a PPP in 11 MS: BE, BG, CZ, ES, FR, HU, IT, NL, PL, RO, SK	http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1799
	Insecticide, acaricide.	
Spatial usage (by MS)	Not in PPP register, not sold as PPP in the 2000's. In Finland the compound is not use.	FI
	Selective contact insecticide and myticide.	RO
	Not approved in SE and DK.	SE; DK
	Uses registered for woody ornamentals.	SK
	Admission for ornamental plants.	BE-FL
Banned uses		
ERC code		
PEC_{fw} (mg/L)		

PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentration

MS	Source of monitoring data	MEC values
In Sc2 (inland whole water) data from 2 MS (785 sites) with 5395 samples are available. All samples are non-quantified. Sc3 was not developed since data scarcity. Data quality is not good.	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.025 µg/l (Sc2) Please note the MEC is not reliable because of the low quantity and quality of monitoring data, and the absence of quantified samples (see column on the left)
UK	Monitored as part of national catchment sensitive farming (CSF) (2 samples per week) & watch list programmes through LC-MS samples at approx. 80 sites.	Only detected once out of the approx. 1700 samples taken at these sites (0.036 µg/l).

Analytical Methods

Pyridaben has been analysed in different food items (Boulaid et al., 2005; Hayward et al., 2015; Hengel and Shibamoto, 2002; Valverde et al., 2002; Zhang et al., 2012).

Wang et al. (2012) analysed 51 pesticides (including pyridaben) and 16 polychlorinated biphenyls (PCBs) in selected fish and food items in Southeast China by gas chromatography tandem mass spectrometry (GC-MS/MS). The results showed that organochlorine pesticides such as DDTs, hexachlorocyclohexanes (HCHs), hexachlorobenzene (HCB) and mirex and other pesticides including chlorpyrifos, pyrethroid pesticides, metolachlor, pyridaben and trifluralin were frequently detected in the samples.

Hakme et al. (2017) have analysed different contaminants (including pyridaben) in honey bees and pollen by gas chromatography time-of-flight mass spectrometry, and the following insecticides/acaricides were detected: chlorpyrifos, coumaphos, fluvalinate-tau, chlorfenvinphos, pyridaben, and propyl cresol.

Method	LOQ (µg/l)	Description / Reference
LC-MS-MS	0.005	LC-MS-MS method for tap, ground and surface water (EFSA, 2010).
LC-MS-MS	0.005 (LOD)	England

P, B, T, C, M, R, ED properties

Substance	Persistent (P) Bioaccumulative (B) Toxic (T)	Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)	Endocrine Disruptive (ED)	Comment
Pyridaben	P and B and T			

Hazard assessment

Ecotoxicology data

Species	Time-scale	Endpoint	Toxicity (µg/L)
Fish			
Pimephales promelas	301 d (flow-through)	NOEC	0.28
Algae			
Skeletonema costatum	120 h (growth rate)	NOEC	8
Invertebrates			
Daphnia magna	21 d (flow-through)	NOEC	0.086
Mysidopsis bahia	35 d (flow-through)	NOEC	0.047
Chironomus riparius	28 d (static)	NOEC	5.1

Data used for PNEC derivation

Source: DAR 2007, RIVM 2008, EFSA 2010 and CLH Report 2013

Mammalian toxicology data

The risk to birds and mammals was assessed as low, after the refinement presented, except for the long-term risk to mammals arising from the use in citrus, where further information is required to address the risk. A high risk was identified for the aquatic environment arising from the use in citrus; no-spray buffer zones up to 30 m were insufficient to address the risk. A high risk was identified for bees for the use in citrus and further information is required. Risk mitigation measures such as 10 m no-spray buffer zones are required to protect non-target arthropods. The risk to earthworms, soil-dwelling macro- and micro-organisms, non-target plants and biological methods of sewage treatment was assessed as low (EFSA, 2010).

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/l)	AF	PNEC value (µg/l)
$PNEC_{fw}$	35-d Reproduction (*M. bahia*)	0.047	10	0.0047
$PNEC_{sed}$				
$PNEC_{biota,secpois}$				
$PNEC_{biota, hh}$				
$PNEC_{dw, hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P(95))/PNEC)	5.3 (Sc2) Please note the RQ(MEC) is highly unreliable because of the low quantity and quality of monitoring data. Exceedancies result from the use of LOQ/2 for the non-quantified samples
RQ_{fw} (PEC/PNEC; PEC=10.4 µg/l)	2212

Note: PEC value is taken from Lettieri, T., Chirico, N., Carvalho, R.N., Napierska, D., Loos, R., Sanseverino, I., Marinov, D., Ceriani, L., Umlauf, G. 2016. *Modelling-based*

strategy for the prioritisation exercise under the Water Framework Directive, https://circabc.europa.eu/w/browse/85b46283-9353-4e67-bf56-e4d18b32cbaf).

STE score

2.11 (Sc2; PNEC=0.0047 µg/l)

Please note the STE score is highly unreliable because of the low quantity and quality of monitoring data. Exceedancies result from the use of LOQ/2 for the non-quantified samples

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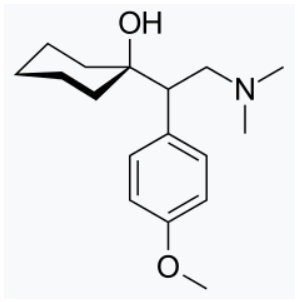
Venlafaxine (CAS N. 93413-69-5)

Substance identity

EC name	
EC number	
CAS number	93413-69-5
Molecular formula	$C_{17}H_{27}NO_2$
Molecular weight	277.4 g/mol
Structure	
SMILES	

Physico-chemical properties

Endpoint	Value	Source
Vapour Pressure (Pa)		
Water solubility (mg/L)	230 g/l	https://www.drugbank.ca/salts/DBSALT000186
logK_{ow}	0.43	http://datasheets.scbt.com/sc-201102.pdf

Environmental fate

Endpoint	Value	Source
Sorption potential K_{oc}		
Partition coefficient solid-water in sediment Kp_{sed} (L/kg)		
Biodegradability		
Bioaccumulation (BCF)		

Environmental exposure assessment

Predicted Environmental Concentration

	Description	Source
Tonnes/year	12	GB
Uses	Antidepressant drug Venlafaxine is used in the following MS: CZ, FI, IRL, RO, SK	
Spatial usage (by MS)	Not known	-
Banned uses		
ERC code		
PEC_{fw} (mg/L)		
PEC_{sed} (mg/kg dw)		
PEC_{biota} (mg/kg)		

Measured Environmental Concentrations

MS	Source of monitoring data	MEC values
Europe (90 samples from 18 countries)	WWTP effluents Loos et al. (2013)	0.119 µg/l (mean) 0.548 µg/l (max.)
DE	WWTP effluents (Germany; DE) Schlüsener et al. (2015)	0.225 µg/l (mean)
DE	Rhine River Schlüsener et al. (2015)	0.014 µg/l (annual mean)
DE	Emscher River (small river) Schlüsener et al. (2015)	0.180 µg/l (mean)
SE	Surface waters downstream WWTPs; also found in blood samples from otters (in 10/10 pooled samples).	<LOQ (0.1 ng/l) up to 0.440 µg/l
In Sc2 (inland whole water) data from only 1 MS (93 sites) with 1395 samples	Dataset of monitoring prioritisation 2014	MEC(P95)= 0.19 µg/l (Sc2)

are available. 76.8% quantified samples. Sc3 was not developed since data scarcity. Data quality is acceptable.		
UK	Monitored at approximately 80 sites (approx. 1700 samples). Detected at 19 of these sites with 15 of these having > 60% detection rate.	0.024-0.49 µg/l (max.) 0.009-0.228 µg/l (mean)

Analytical Methods

Method	**LOQ (µg/l)**	**Description / Reference**
SPE-LC-MS-MS	0.0007	Extraction of 100 ml water (Gros et al. (2012)
SPE-LC-MS-MS	0.0005	Extraction of 100 ml water (Loos et al. (2013)
SPE-LC-MS-MS	0.0003	Extraction of 1 L water (Schlüsener et al.; 2015)
LC-MS-MS	0.01	CZ
n.a.	0.0001	SE
n.a.	0.0005	BE-Wallonia
LC-MS-MS	0.005	England

P, B, T, C, M, R, ED properties

Substance	**Persistent (P) Bioaccumulative (B) Toxic (T)**	**Carcinogenic (C) Mutagenic (M) Reproduction toxicity (R)**	**Endocrine Disruptive (ED)**	**Comment**
Venlafaxine	P and T			

Hazard assessment

Ecotoxicology data

Mammalian toxicology data

PNEC derivation

PNEC	Endpoint	Endpoint value (µg/L)	AF	PNEC value (µg/L)
$PNEC_{fw}$				0.038
$PNEC_{sed}$				
$PNEC_{biota,sec\ pois}$				
$PNEC_{biota,\ hh}$				
$PNEC_{dw,\ hh}$				

Risk Quotient (MEC or PEC/PNEC)

RQ	Value
RQ_{fw} (MEC(P95)/PNEC)	
RQ_{fw}(PEC/PNEC; PEC=0.2 µg/l)	
RQ_{sed}	
$RQ_{biota,sec\ pois}$	
$RQ_{biota,\ hh}$	
$RQ_{dw,\ hh}$	

STE score

n.a.

References

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